A novel, environment-friendly method to prepare pyranones from furfural alcohols via photocatalytic O_2 oxidation in an aqueous phase

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Electronic Supplementary Information

Contents

1. General experiment

1.1 Experiment

Photocatalysis experiments were performed in an argon or oxygen atmosphere. Chemical reagents (including purified water) were obtained from commercial suppliers (*Sigma-Aldrich, Adamas,* Shanghai Titan Technology Co., LTD, et al.) and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) on a 0.25 mm silica gel GF254 plate (Merck Silica gel 60-F254) using UV light as a visualizing agent and an ethanolic solution of phosphomolybdic acid and cerium sulfate and heat as a developing agent. Silica gel (300-400 mesh) was used for normal flash column chromatography. Pyranone and its related derivate products were isolated by column chromatography with neutral alumina (Al_2O_3, Merck KGaA, 70–230 mesh, and pH = 6.8–7.8). Ethyl acetate and petroleum ether were used as the eluent solvents. Yields refer to chromatographically and spectroscopically homogeneous materials unless otherwise noted. **LED lights** (including 18W LEDs with different wavenumbers) were purchased from the Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, and Changchun Changguang Chenpu Technology Co., LTD. **React IR 15^{TM}** from Mettler-Toledo Auto Chem. company was employed for the *in-situ* reaction kinetic experiments. The reaction spectra were recorded by using iC IR software, version 7.1.

1.2 Analysis

EPR spectra were recorded at room temperature on a Bruker EMX micro A300 spectrometer operated at 9.8543 GHz.

^{1}H-NMR, and **^{13}C-NMR** were recorded with Bruker Advance (400 and 500 MHz) spectrometers. All chemical shifts were reported as δ values in parts per million (ppm) and coupling constants (J) in Hz. Tetramethylsilane (TMS) was used as the internal standard for $CDCl_3$ (7.26 ppm for ^{1}H, 77.00 ppm for ^{13}C).

Mass spectra: **(1)** ***HR-MS (ESI)*** was taken on AB QSTAR Pulsar mass spectrometer or Agilent LC/MSD TOF mass spectrometer. HR-MS data were recorded via electron impact mass spectrometry using a time-of-flight analyzer. ***(2) GC–MS*** was performed on a Hewlett-Packard 6890 N gas chromatograph (equipped with the same HP-5MS capillary column) under identical operating conditions used in Mass Spectral Library by R. P. Adams (Adams, 2007).

Electrochemistry: cyclic voltammograms (CVs) were obtained on a Metrohm PGSTAT302N potentiostat.

UV-Visible (UV-VIS) absorption measurements were collected and analyzed using an Agilent Cary 5000 spectrophotometer.

Fluorescence (FL) emission intensities experiments were conducted on a Hitachi F-4600 luminescence Spectrophotometer.

1.3 Biosynthetic pathway from lignocellulose to biomass furans

The biological transformation pathway from biomass lignocellulose to glucoses, furans, and short-chained alcohol acid (including alcohols, acids, and lactones), as demonstrated in ***Figure S1***.[1]

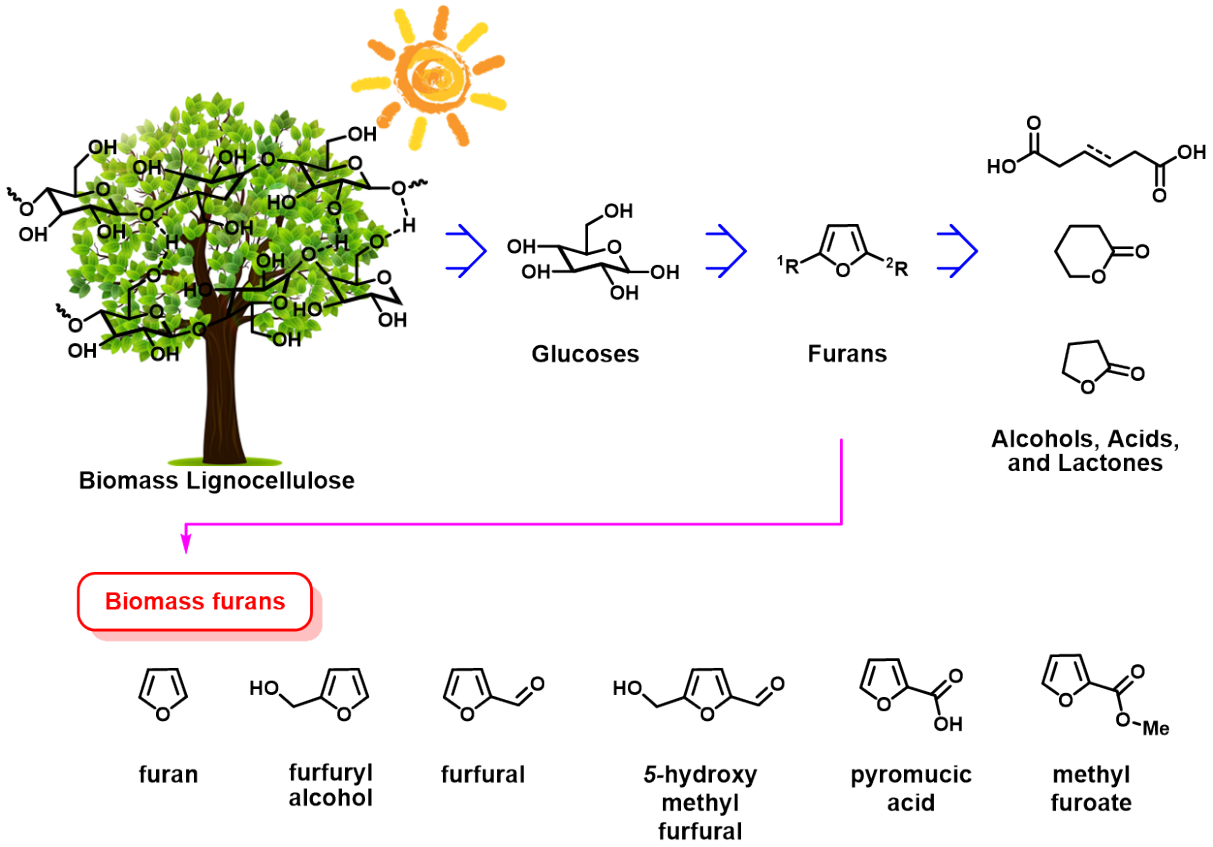
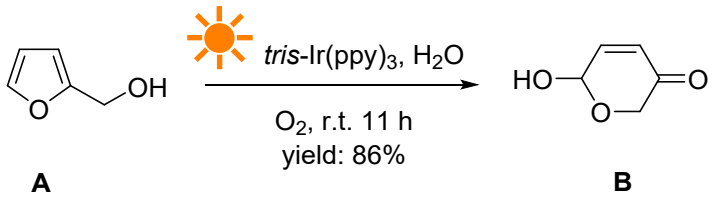


Figure S1. Biological transformation pathway of biomass.

2. Basic Photocatalysis experiment

2.1 General photocatalysis



A **B**

In an oven-dried quartz flask (25 mL) equipped with a stir bar, furfuryl alcohol (500 mg, 5.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (7.3 mg, 0.1 mmol, 0.002 equiv.), and H_2O (10.0 mL) were combined and added. The reaction was conducted under an oxygen atmosphere using an O_2 balloon. The reaction mixture was stirred and illuminated by two 18 W visible LED lights (a total of 36 W) under room temperature for 11 h cooling by a fan. TLC, UV light as a visualizing agent, the reaction was monitored, and an ethanolic solution of phosphomolybdic acid, cerium sulfate, and heat as a developing agent. When the reactant material was no longer decreased, the solution was extracted with EtOAc (3×10 mL) and H_2O (3×10 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on neutral alumina (Al_2O_3, Merck KGaA, 70–230 mesh, and pH = 6.8–7.8) using ethyl acetate and petroleum ether (5:1, vol/vol) as the eluent solvents. The 6-hydroxy-2H-pyran-3(6H)-one (pyranone product) **B** was obtained in a yield of 421.4 mg, 86%, with a conversion efficiency of 90%. All the pyranone products isolated yield by column chromatography with neutral alumina, Al_2O_3, Merck KGaA, 70–230 mesh, and pH = 6.8–7.8 as the ideal medium.

The reaction Yield and Conversion Efficiency were calculated by using ***Equation S1*** and ***Equation S2***, as below:

$$Yield\ (\%) = \frac{mole\ of\ product\ obtained}{mole\ of\ reactant\ consumed} \times 100\% \qquad (\boldsymbol{S1})$$

$$Conversion\ Efficiency\ (\%) = \frac{mole\ of\ reactant\ consumed}{mole\ of\ reactant\ before\ reaction} \times 100\% \qquad (\boldsymbol{S2})$$

The Turnover Frequency (TOF) of the photocatalyst was calculated at room temperature of 25 °C, and based on ***Equation S3***, as below:

$$TOF = \frac{mole\ of\ product\ formed}{mole\ of\ metal\ catalyst\ used \times reaction\ time} \times 100\% \qquad (\boldsymbol{S3})$$

2.2 Different light wave reactions

Seven standard reaction mixtures in 10-mL vials were charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), and H_2O (5.0 mL), the vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction mixture was degassed by oxygen sparging for 10 min. It was conducted under an oxygen atmosphere using an O_2 balloon, importantly, irradiated with 18 W visible LEDs lamps with seven different wave numbers (365-370nm, 395-400nm, 410-415nm, 460-465nm, 520-525nm, 590-595nm, 620-625nm), and cooling by a fan. After 2 h, the lamps were turned off, and one vial was removed from the irradiation setup for analysis. The gas chromatography (GC) measurements were employed for the yield and conversion efficiency analysis, as demonstrated below:

Wavelength	365 ~ 370	395 ~ 400	410 ~ 415	460 ~ 465	520 ~ 525	590 ~ 595	620 ~ 625
Yield (%)	12	16	20	40	58	70	75
Conversion Efficiency (%)	70	65	60	55	34	20	12

Table S1. Effect of light wavelength on reaction yield and conversion efficiency.

2.3 The 10.00 gram-scale reaction

In an oven-dried quartz flask (250 mL) equipped with a stir bar, furfuryl alcohol (10.0 g, 102.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (36.5 mg, 0.051 mmol, 0.0005 equiv.), and H_2O (100.0 mL) were combined and added. The reaction was conducted under an oxygen atmosphere using an O_2 balloon. The reaction mixture was stirred and illuminated by four 18 W visible LED lights (a total of 72 W) under room temperature for 48 h cooling by a fan. TLC, UV light as a visualizing agent, the reaction was monitored, and an ethanolic solution of phosphomolybdic acid, cerium sulfate, and heat as a developing agent. When the reactant material was no longer decreased, the solution was extracted with EtOAc (3×50 mL) and H_2O (3×50 mL). The combined organic layer was dried with Na_2SO_4 and filtered. The solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on neutral alumina (Al_2O_3, Merck KGaA, 70–230 mesh, and pH = 6.8–7.8) using ethyl acetate and petroleum ether (5:1, vol/vol) as the eluent solvents. The 6-hydroxy-2H-pyran-3(6H)-one (pyranone product) **B** was obtained in a yield of 7.735g, 79%, with a conversion efficiency of 85%.

3. *In-situ* IR experiment

3.1 General *in-situ* IR experiment and photocatalysis apparatus

For the operando IR kinetic experiments, the reaction spectra were recorded using an IC 15 from Mettler-Toledo Auto Chem. Data manipulation was carried out using the iC IR software, version 7.1. **React IR 15™**, Detector: MCT, Apodization: HappGenzel, Probe: DiComp (Diamond), Interface: AgX 6 mm * 1.5 m Fiber (Silver Halide), Sampling: 3000 to 650 cm^{-1}.

The reaction was carried out as follows: a three-neck reaction vessel was fitted with a magnetic stirring bar. The MIR ATR IR probe was inserted into the middle neck through an adapter. Septa capped the other two necks for injections and an atmosphere line. Following evacuation in a vacuum and flushing with oxygen three times, the three-neck vessel was charged with a solution of reactants. The reaction conditions were 25 °C and used an oxygen balloon atmosphere, with water as the solvent. Operando IR spectra were recorded throughout the reaction.

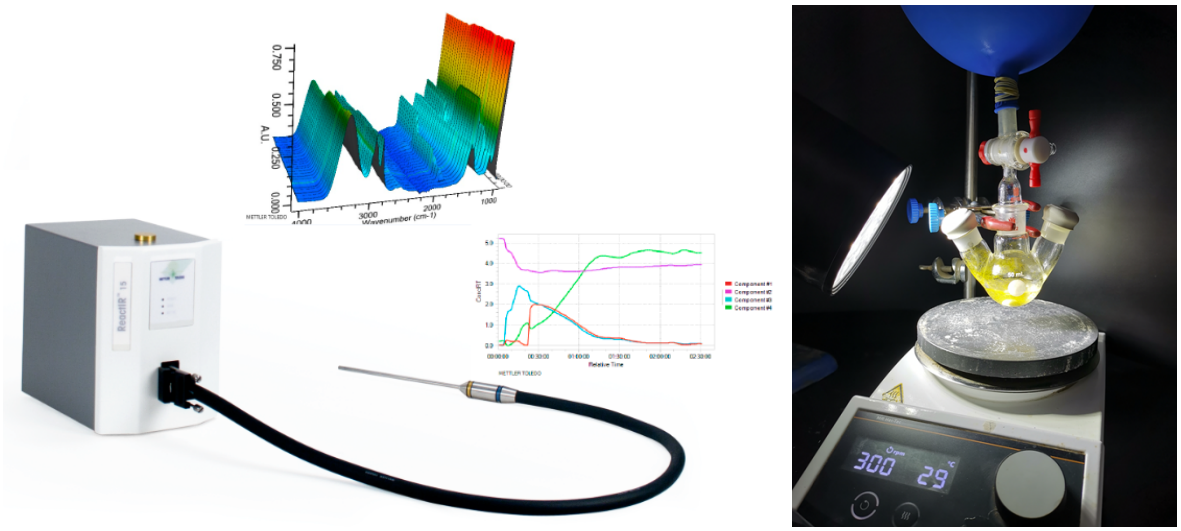


Figure S2. MIR trends for all the key reaction species and their relative concentrations throughout the reaction.

3.2 React IR Experimental data

The concentration of furfuryl alcohol was monitored by ConcIRT at 2950 cm^{-1}, and ConcIRT monitored the concentration of the pyranone product at 1500 cm^{-1}. React IR experimental data for the photocatalysis progress was collected from the original data every 30 min, as shown in the table below.

Table S2. React IR Experimental data (recorded every 30 min).

No.	time (/ 30 min)	[reactant] * 100	[product] * 100	(C/C_0)	ln (C/C_0)	-ln [product]
1	26.67	9.55	0.0117	1.0000	0.000000	4.4447
2	56.67	9.38	0.0120	0.9815	-0.018691	4.4258
3	86.67	9.14	0.0179	0.9571	-0.043840	4.0254
4	116.67	9.01	0.0269	0.9428	-0.058852	3.6173
5	146.67	8.91	0.0333	0.9324	-0.070003	3.4008
6	176.68	8.78	0.0404	0.9196	-0.083789	3.2089
7	206.68	8.61	0.0528	0.9010	-0.104234	2.9420
8	236.68	8.35	0.0625	0.8744	-0.134174	2.7731
9	266.68	8.19	0.0731	0.8572	-0.154096	2.6161
10	296.68	8.14	0.0855	0.8518	-0.160422	2.4591
11	326.68	7.83	0.0975	0.8200	-0.198487	2.3276
12	356.68	7.67	0.1048	0.8033	-0.218976	2.2558
13	386.68	7.41	0.1166	0.7761	-0.253461	2.1489
14	416.68	7.21	0.1328	0.7549	-0.281219	2.0186
15	446.68	7.23	0.1231	0.7573	-0.277982	2.0944
16	476.70	7.11	0.1275	0.7442	-0.295430	2.0598
17	506.70	6.85	0.1449	0.7168	-0.332969	1.9320
18	536.70	6.50	0.1703	0.6800	-0.385647	1.7701
19	566.70	6.11	0.1870	0.6400	-0.446293	1.6764
20	596.70	5.82	0.2079	0.6097	-0.494808	1.5705
21	626.70	5.85	0.2074	0.6127	-0.489895	1.5730
22	656.70	5.64	0.2179	0.5903	-0.527068	1.5235
23	686.70	5.53	0.2310	0.5791	-0.546195	1.4652
24	695.53	5.67	0.2206	0.5939	-0.520996	1.5113

(A) *k* and R of the reaction with [FAL] varied in the range of 1.5-3.25 mol·L^{-1}.

[FAL] mol·L^{-1}	**0.5**	**1.5**	**2.5**	**3.25**
k	8	7.7	8.1	8.2
R	5.6	5.7	5.7	5.6

(B) reaction progress with different [*tris*-Ir(*ppy*)$_3$].

[Ir] (mol-%)	**1.0**	**0.2**	**0.1**	**0.01**
k	8	7.8	7.5	2.1
R	5.6	5.5	5.6	5.6

(C) impact of different white light power on *k* and R.

Light intensity (W)	**18**	**36**	**54**	**72**
k	8	8.2	7.9	7.2
R	5.6	5.5	5.2	5.8

(D) impact of different reaction atmospheres on *k* and R.

reaction atmosphere	**O_2 ballon**	**air**	**Argon**	**Quinone (2.0 equiv.)**
k	8	2.8	--	14.5
R	5.6	5.2	--	5.9

3.3 NMR monitoring for reaction progress

An important furan-[O] intermediate was detected in this photocatalysis reaction by using ^{1}H-NMR experiment tests. As shown in ***Figure S3***, the signal of a furan-[O] intermediate was created and accumulated in the first hour of furan oxidation (***process A***), then the concentration decreased with the furan-ring arrangement (***process B***) and finally vanished at the end. ^{1}H-NMR measurements at different reaction times were conducted to capture the intermediate during the reaction. As demonstrated in the ^{1}H-NMR map, a clear C=C bond migration signal was observed at the chemical shift of λ = 7.5 ~ 8.0, which could be explained by the structure change of the C=C bond in furan rings. At the same time, the C=C bond migration signal increased notably when the reaction was conducted in an O_2 atmosphere.

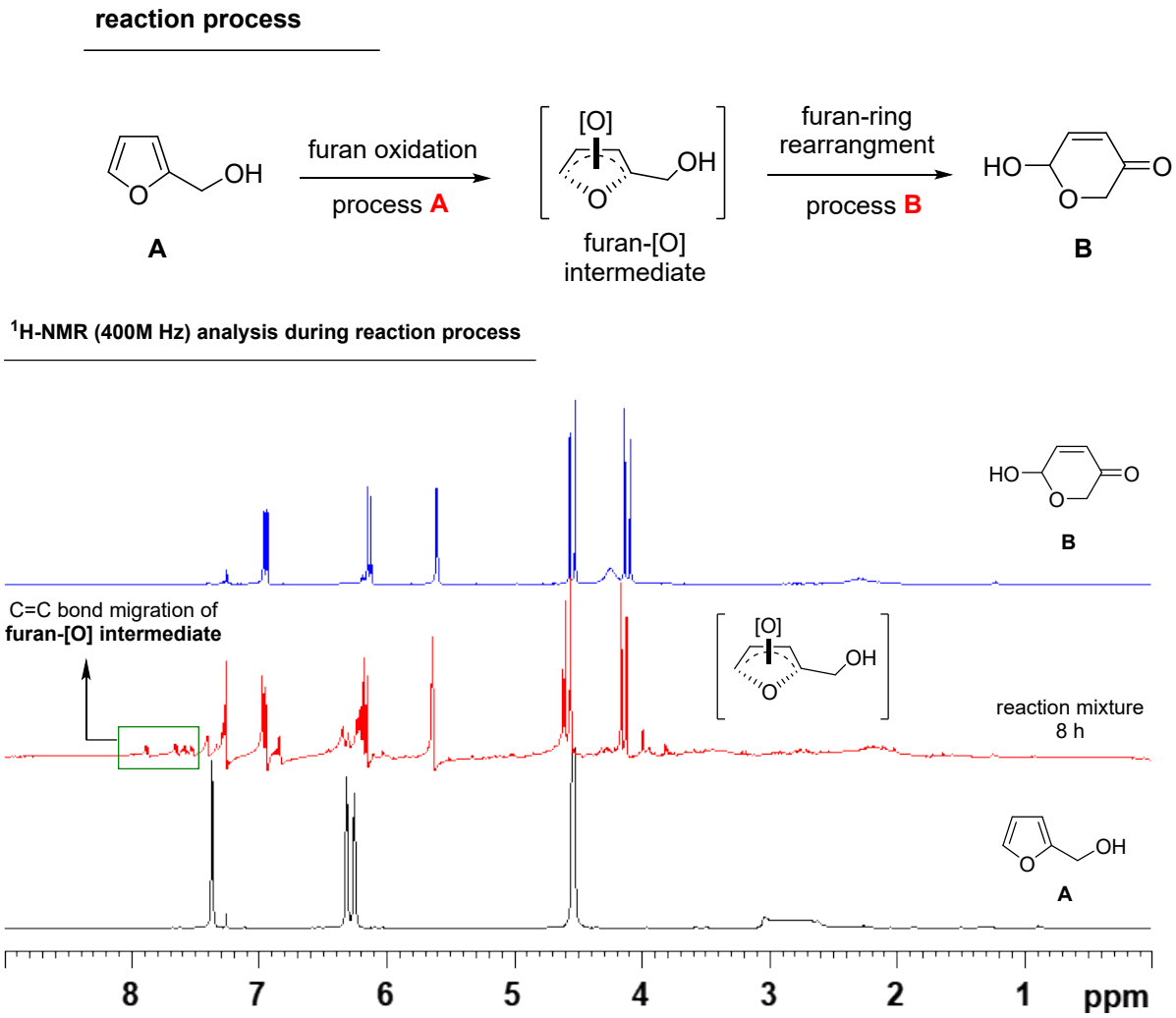


Figure S3. ^{1}H-NMR spectra for reactant **A**, **furan-[O] intermediate** was detected of the reaction solution over a reaction time of 8 h, and NMR of product **B**.

4. Mechanistic investigations

4.1 Radical inhibition experiments

A standard reaction mixture in 10-mL vials was charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), and H_2O (5.0 mL), the vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction was conducted under an oxygen atmosphere using an O_2 balloon. Additionally, to test the radical inhabitation of this electrocatalysis experiment, a chemical equivalent of TEMPO, butylated hydroxytoluene, or $^{n}Bu_3SnH$ was added to the reaction solutions. The reaction mixture was degassed by oxygen sparging for 10 min, irradiated with 18 W visible LED lamps, and cooled by a fan. The reaction was monitored by TLC, UV light as a visualizing agent, and an ethanolic solution of phosphomolybdic acid, cerium sulfate, and heat as a developing agent. GC-MS tested the photocatalytic reactions to detect pyranone products. GC-MS captured the TEMPO-pyridyl adduct product with a molecular weight of 311, and its yield was tested by GC at 38%.

4.2 EPR spin-trapping experiments

EPR spectra were recorded at room temperature on a Bruker EMX micro A300 spectrometer operated at 9.8543 GHz. Typical spectrometer parameters are shown as follows, sweep width: 6000 G; center field set: 3000 G; time constant: 81.92 ms; sweep time: 327.68 s, modulation amplitude: 1.00 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^3; microwave power: 18.53 mW.

EPR experiment for photocatalysis

A standard reaction mixture in 10-mL vials was charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), and H_2O (5.0 mL), the vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction was conducted under an oxygen atmosphere using an O_2 balloon. The reaction mixture was stirred and illuminated by two 18 W visible LED lights (a total of 36 W) at room temperature and cooling by a fan. The reaction mixture was syringed out, combined with a TEMP ($2.0\ mol\cdot L^{-1}$) solution, and repeated the test procedure three times: (1) before photo-irradiation, (2) photo-irradiation about 10 min, and (3) photo-irradiation about 30 min. Then the EPR signals were recorded and calculated.

4.3 Light ON/OFF experiments

Seven standard reaction mixtures in 10-mL vials were charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), and H_2O (5.0 mL), the vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction mixture was degassed by oxygen sparging for 10 min. It was conducted under an oxygen atmosphere using an O_2 balloon, then irradiated with 18 W visible LED lamps and cooled by a fan. After 2 h, the lamps were turned off, and one vial was removed from the irradiation setup for analysis. The remaining six vials were stirred without light for an additional 1 h. Then, one vial was removed for analysis, and the lamps were turned back on to irradiate the remaining five reaction mixtures. After an additional 2 h of irradiation, the lamps were turned off, and one vial was removed for analysis. The remaining four vials were stirred without light for an additional 1 h. Then, a vial was removed for analysis, and the lamps were turned back on to irradiate the remaining three reaction mixtures. After 2 h, the lamps were turned off, and one vial was removed for analysis. The remaining two vials were stirred in the absence of light.

4.4 Measurement of quantum yield experiments

The experiments for measurement of quantum yield were conducted by using the spectrometer of Thorlabs Optical Power/Energy Meter: Model S310C. The light intensity was 9.3 mW·cm^{-2}, the LED light source was 18 W, and the reactions were conducted over a time of 2 h. the $^1O_2$ photocatalysis quantum yield was calculated as 11%, by using ***Equation S4*** as below:[2, 3]

$$\Phi so\ (\%) = \frac{Ne}{Np} \times 100\% \qquad (\boldsymbol{S4})$$

Φso: Quantum Yield, Ne: reactive photons per second, Np: absorbed photons per second.

$$Ne = vtNA \times 100\%$$

v: the average photocatalysis reaction rate (mol·s^{-1}), t: irradiation time (s), N_A is Avogadro's constant, 6.02×10^{23} (mol^{-1}).[4]

$$Np = \frac{IAt\lambda}{hc} \times 100\%$$

I: Optical power density of incident light (W·m^{-2}), A: irradiation area (m^2), λ: wavelength of incident rays (nm), t: time (s), h: Planck constant (6.62×10^{-34} J·s), c: the speed of light (3.0×10^8 m·s^{-1}).[5]

Table S3. Photocatalysis reaction data

No.	Reactant (mg)	Photocatalyst (mg)	Solvent (mL)	Yield (%)	Reaction time (h)	Light power (W)
1	75	5	5	13	2	18
2	75	5	5	17	2	18
3	75	5	5	15	2	18

4.5 Isotope-Labeling experiments

Two standard reaction mixtures in 10-mL vials were charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine), iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), using $\mathbf{D}_2O$ or $H_2{}^{\mathbf{18}}\mathbf{O}$ (5.0 mL) as the solvent, the two vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction mixtures were degassed by oxygen sparging for 10 min. They were conducted under an oxygen atmosphere using an O_2 balloon., then irradiated with 18 W visible LED lamps and cooled by fans.

(1) In the $H_2{}^{\mathbf{18}}\mathbf{O}$ experiment, pyranone product was detected with a molecular weight of 114, and no $^{\mathbf{18}}\mathbf{O}$ atom was involved. (2) In the $\mathbf{D}_2O$ experiment, a deuterated **D**-pyranone product was detected with a molecular weight of 115.

4.6 GC-MS analysis for no H_2O solvent experiment

A standard reaction mixture in 10-mL vials was charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine) iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), especially with no water solvent added. The reaction was conducted under an oxygen atmosphere using an O_2 balloon. The vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction mixture was degassed by oxygen sparging for 10 min, irradiated with 18 W visible LED lamps, and cooled by a fan. After a photo-irradiation of about 1 h, the reaction mixture was analyzed by GC-MS. Reaction products of aldehyde, acid, and furan-one were detected.

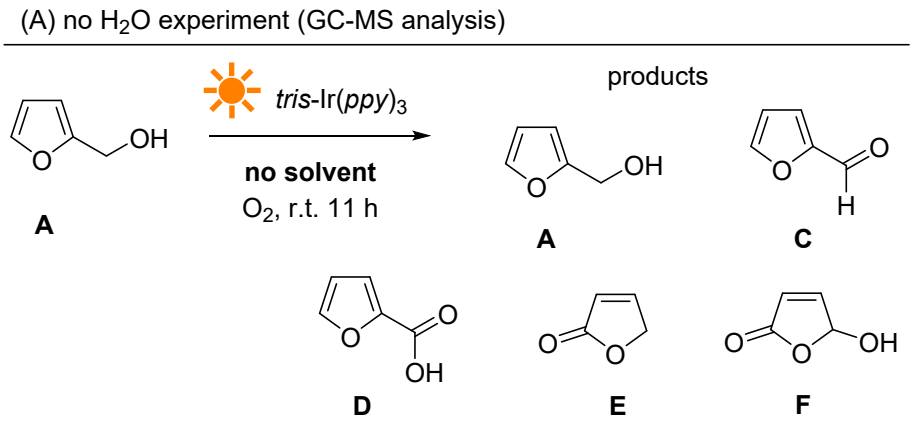
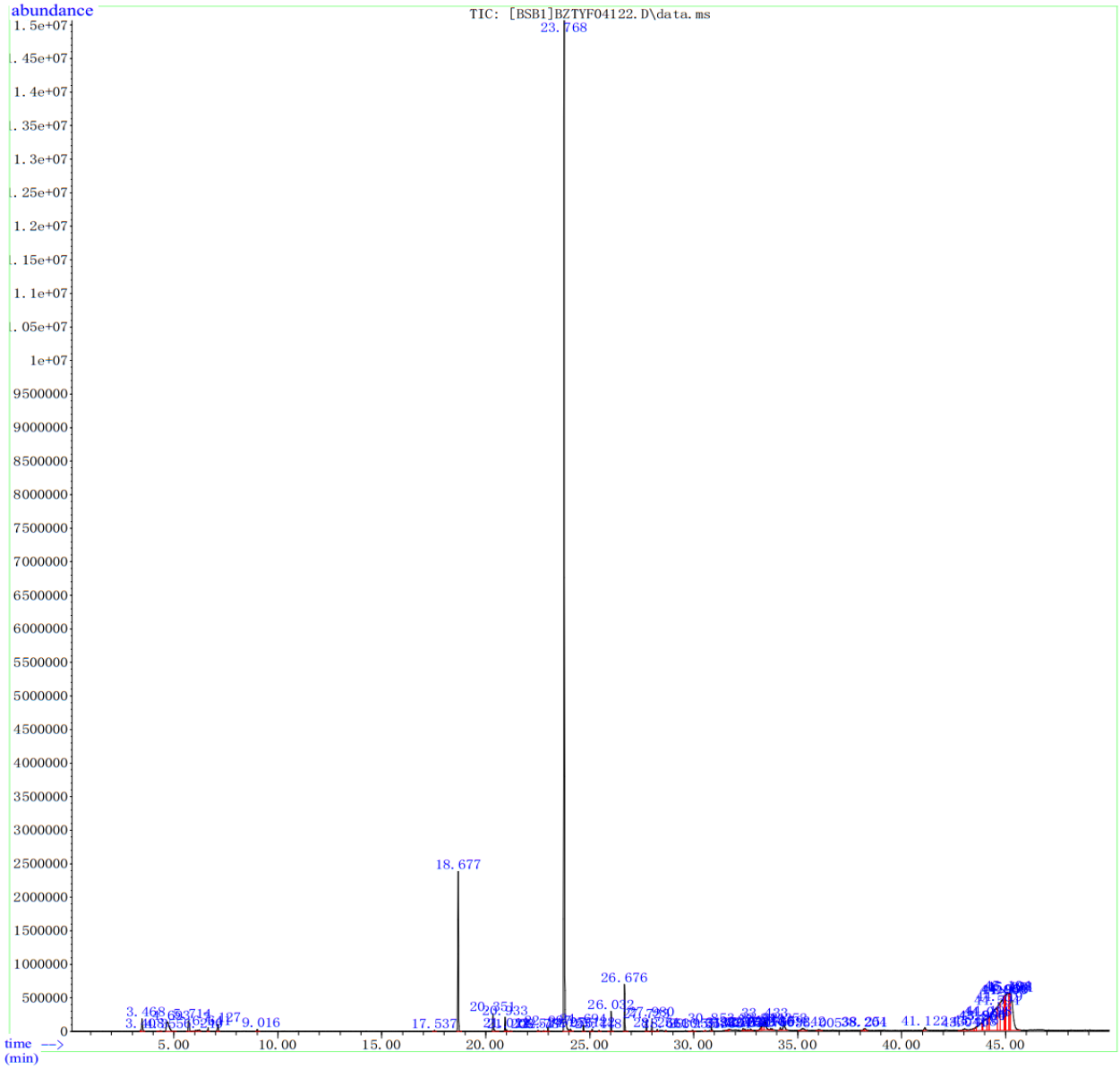


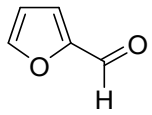
Figure S4. GC-MS analysis of the photocatalysis experiment without H_2O.

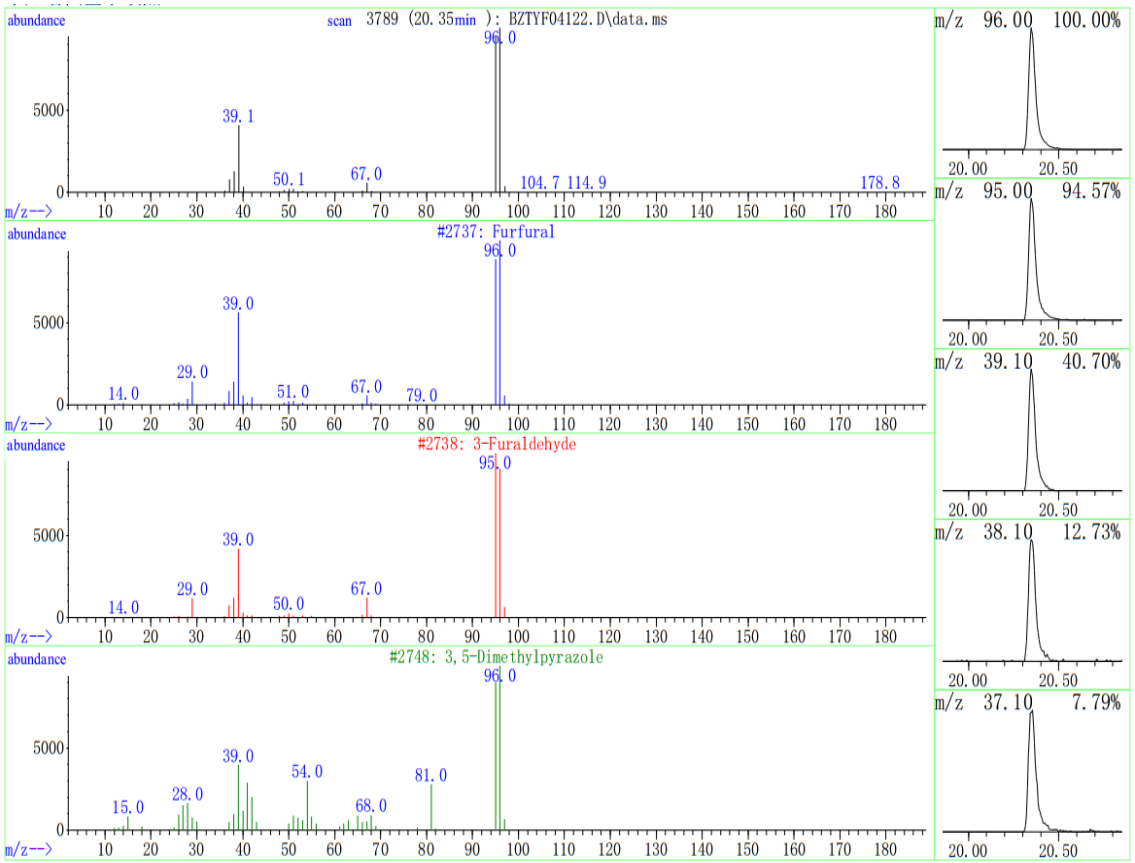
GC-MS spectroscopy

1. The full map



2. product furaldehyde





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sample-1

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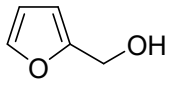
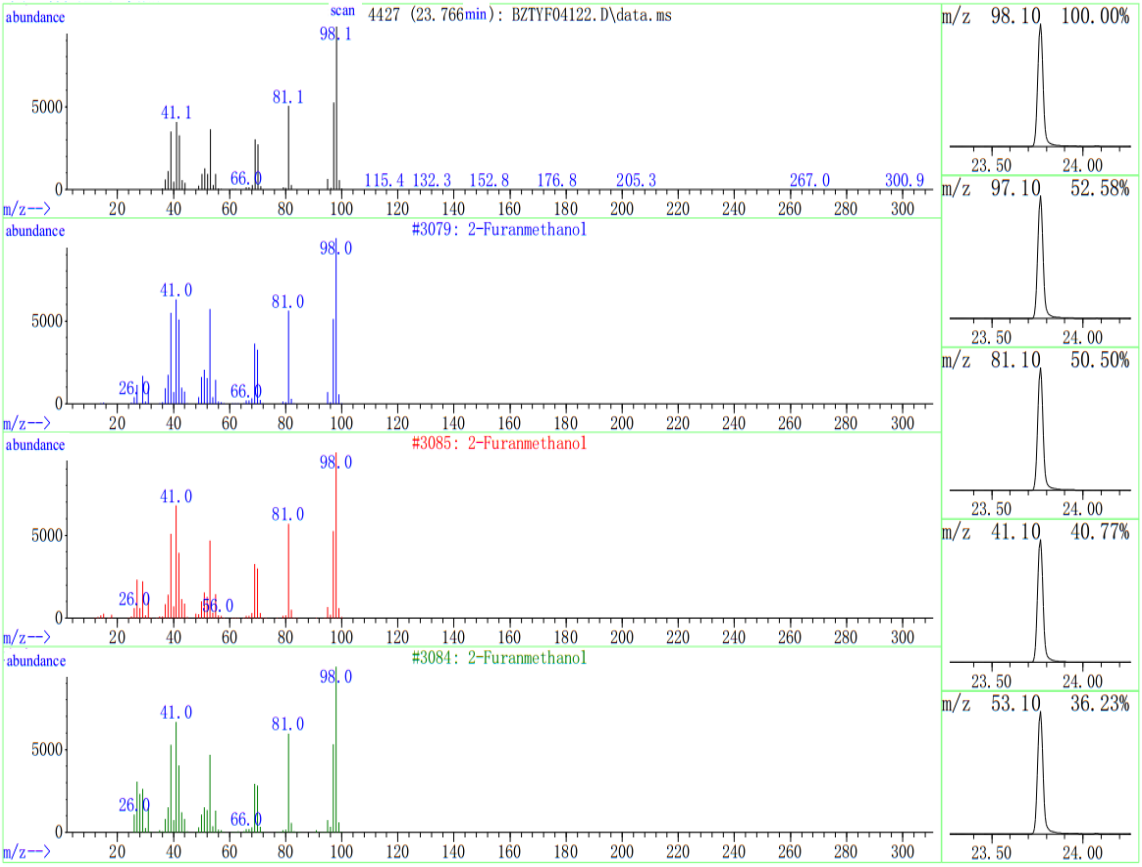
2 3-Furaldehyde	2738	000498-60-2	90
3 3,5-Dimethylpyrazole	2748	000067-51-6	64

3. reactant furfuryl alcohol





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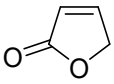

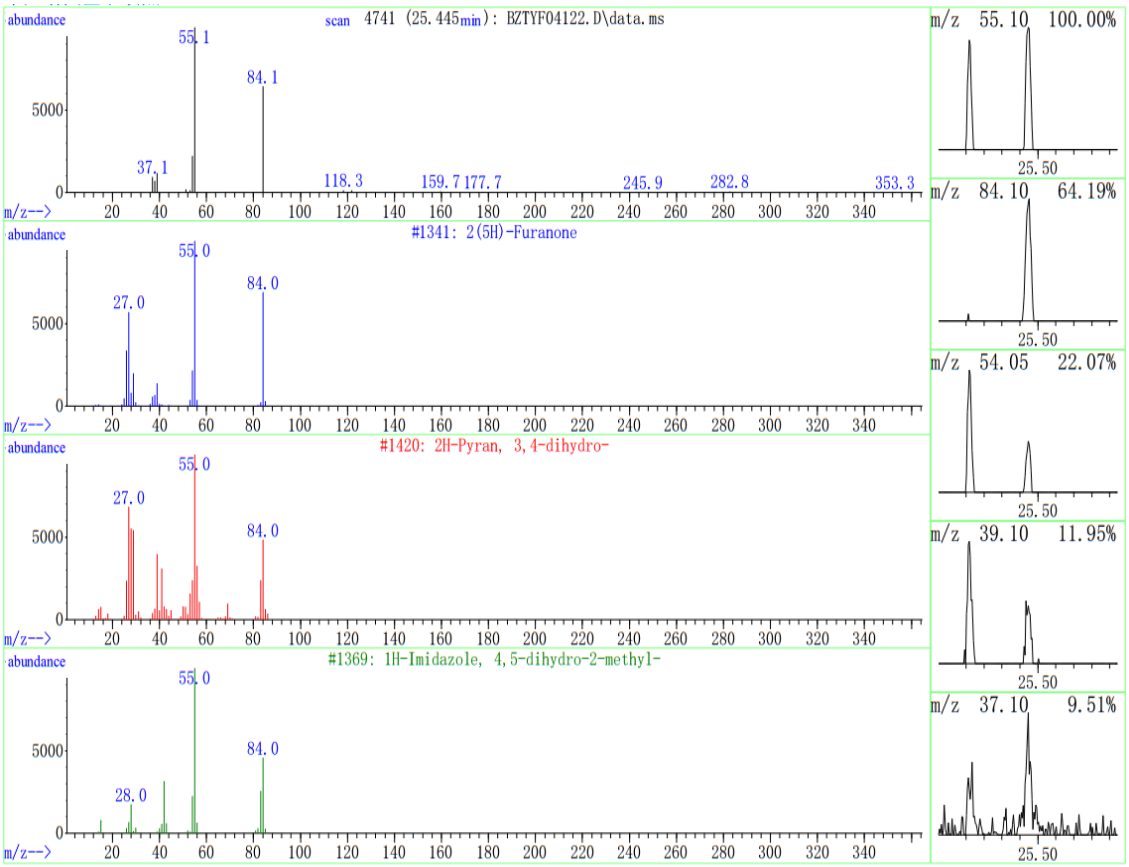

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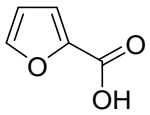
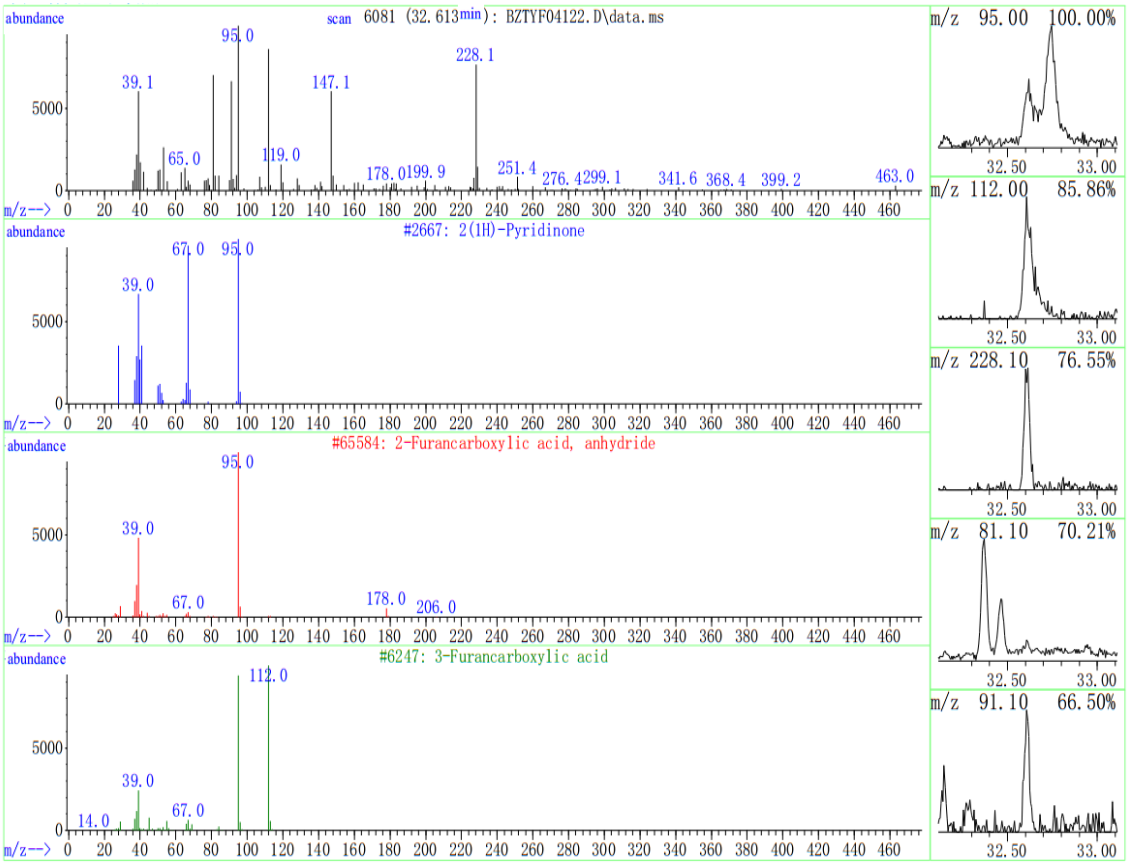
3 1H-Imidazole, 4,5-dihydro-2-methyl-	1369	000534-26-9	9

5. product furancarboxylic acid





Data File: C:\msdchem\2\data\2022\20220426-2204229278 \BSB\BZTYF04122.D
sample-1

No. 37 32.613 min area 449604 area % 0.06

3 best compounds of library	Ref\#	CAS\#	matching rate
C:\Database\NIST11.L			
1 2(1H)-Pyridinone	2667	000142-08-5	38
2 2-Furancarboxylic acid, anhydride	65584	000615-08-7	38
3 3-Furancarboxylic acid	6247	000488-93-7	38

4.7 GC-MS analysis for no O_2 atmosphere experiment

A standard reaction mixture in 10-mL vials was charged with furfuryl alcohol (100 mg, 1.0 mmol, 1.0 equiv.), *tris*-(*2*-phenylpyridine), iridium (6.5 mg, 0.01 mmol, 0.01 equiv.), with no water solvent (10 mL) added, the vials were sealed with poly-tetrafluoro-ethylene-lined caps. The reaction mixture was degassed by argon sparging for 10 min. The reaction was conducted in an oxygen atmosphere using an Ar balloon. Then irradiated with 18 W visible LED lamps and cooled by a fan. After a photo-irradiation about 1 h, the reaction mixture was analyzed by GC-MS. Almost all reactant was detected in the reaction mixture.

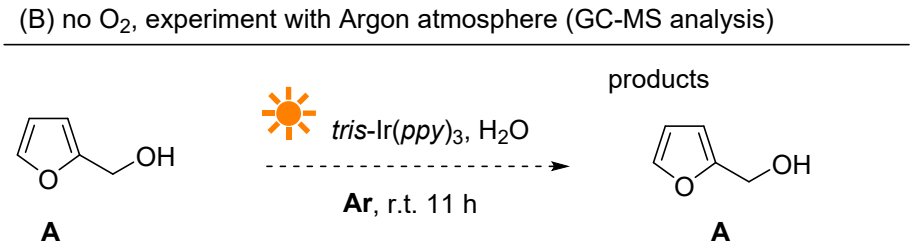
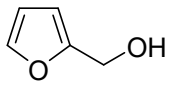
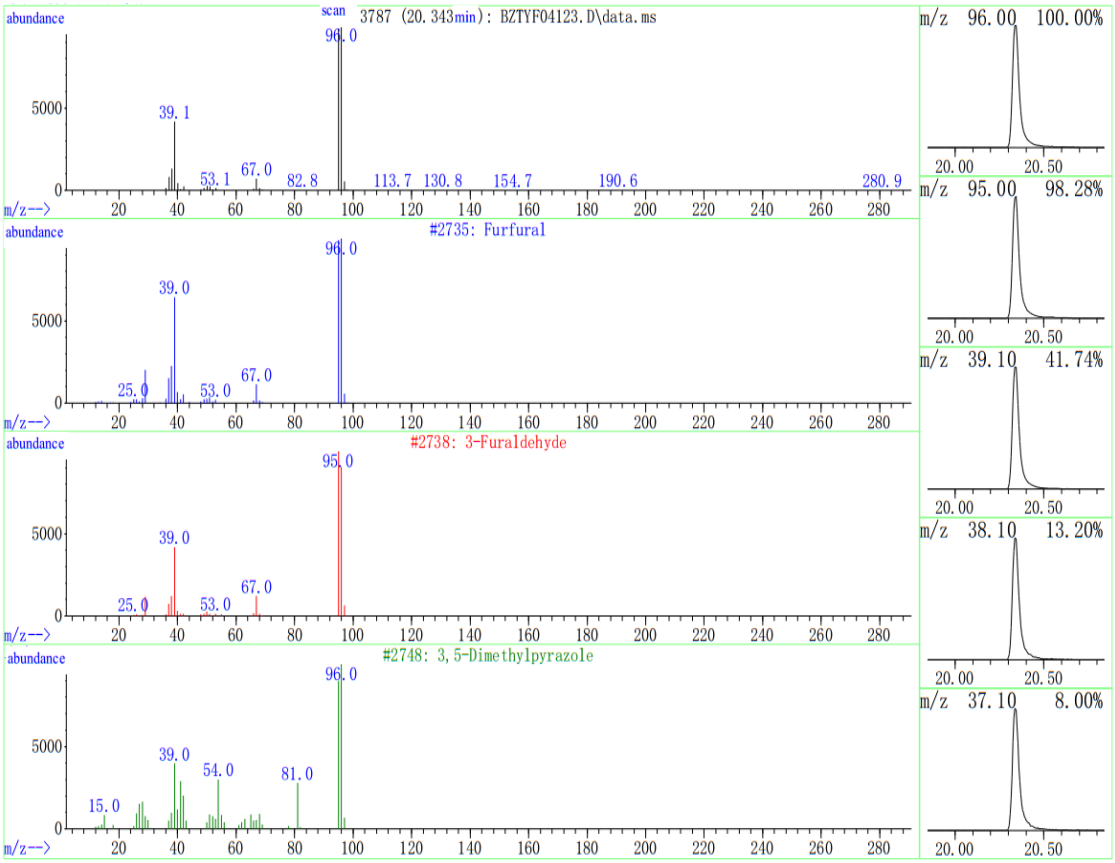


Figure S5. GC-MS analysis of the photocatalysis experiment without O_2.

GC-MS spectroscopy

1. reactant furfuryl alcohol





Data File: C:\msdchem\2\data\2022\20220426-2204229278 \BSB\BZTYF04123.D
sample-2

No. 7 20.343 min area 42637952 area % 1.34

3 best compounds of library	Ref\#	CAS\#	matching rate
C:\Database\NIST11.L			
1 Furfural	2735	000098-01-1	94
2 3-Furaldehyde	2738	000498-60-2	91
3 3,5-Dimethylpyrazole	2748	000067-51-6	83

4.8 UV-VIS experiments

UV-Visible absorption measurements were collected and analyzed using an Agilent Cary 5000 spectrophotometer. Solutions of different furfuryl alcohol and *tris*-(*2*-phenylpyridine) iridium were introduced to a 1 cm path length quartz cuvette equipped with a Teflon® septum under an argon atmosphere (all solutions were prepared in the dark).

For the solutions of furfuryl alcohol in H_2O with an **O_2 atmosphere**: furfuryl alcohol (5 mg, 0.05 mmol), and *tris*-Ir(*ppy*)$_3$ (0.5 mg, 0.00075 mmol) were dissolved in H_2O (5 mL) under O_2 atmosphere, the reaction mixtures were photo-irradiated under visible light about 0 h, 0.5 h, 1 h, 3 h, 5 h, 7 h, and 11 h, then reaction mixtures were separately transformed to 1 cm length quartz cuvettes, sealed with Teflon® septa, and then tested with a stream of oxygen.

For the solutions of furfuryl alcohol in H_2O with **Ar atmosphere**: furfuryl alcohol (5 mg, 0.05 mmol), and *tris*-Ir(*ppy*)$_3$ (0.5 mg, 0.00075 mmol) were dissolved in H_2O (5 mL) and degassed with a stream of argon for 10 minutes, the reaction mixtures were photo-irradiated under visible light about 0 h, 0.5 h, 1 h, and 11 h, then reaction mixtures were separately transformed to 1 cm length quartz cuvettes, sealed with Teflon® septa, and tested.

4.9 Fluorescence experiments

Fluorescence (FL) emission intensities experiments were conducted on a Hitachi F-4600 luminescence Spectrophotometer. All solutions of different furfuryl alcohol and *tris*-(*2*-phenylpyridine) iridium were excited at 260 nm, a pitch of 5 nm, and the emission intensity was collected at 275 nm. The scan rate was 12000 $nm \cdot min^{-1,}$ and the photomultiplier tube voltage (PTV) was 680 V. The light source for fluorescence lifetime measurement was a 380 EPL TCSPC laser with an increment of 1.0 nm and a monochromatic band of 2.0 nm.

For two solutions of furfuryl alcohol in H_2O with **O_2 atmosphere** or **Ar atmosphere**: furfuryl alcohol (5 mg, 0.05 mmol) and *tris*-Ir(*ppy*)$_3$ (0.5 mg, 0.00075 mmol) were dissolved in H_2O (5 mL) under O_2 (or **Ar)** atmosphere, the reaction mixtures were photo-irradiated under visible light about 11 h, then reaction mixtures were separately transformed to 1 cm length quartz cuvettes, sealed with Teflon® septa, and then tested with a stream of Ar.

4.10 Stern−Volmer fluorescence quenching experiments

Stern-Volmer experiments were conducted on a Hitachi F-4600 Fluorescence Luminescence Spectrophotometer. Each component was prepared in H_2O prior to each set of experiments. The solutions were irradiated at λex = 270 nm, and the luminescence was measured at λem = 290 nm. To set up the Stern-Volmer graph, plot the concentration of furfuryl alcohol reactant, [Q], on the x-axis and I_0/I_f on the y-axis according to ***Equation S5***:[6]

$$\frac{Io}{If} = 1 + Ksv[Q] \qquad (\boldsymbol{S5})$$

I_0 and I_f are the luminescence intensities in the absence and presence of furfuryl alcohol. The slope of the Stern-Volmer graph, K_{sv} can be used to compare quenching efficiencies using the assumption that adding quencher (furfuryl alcohol reactant) into the solution does not change the luminophore natural rate of decay ($k_q = k_o$). The value for I_0/I_f from each run was averaged to yield a value of I_0/I_f for the experiment. Linear regression of I_0/I_f against concentration was performed in Origin.

Table S4. Stern−Volmer fluorescence quenching experiments data

reactant and photocatalyst	**Concentration (mM)**
tris-Ir(*ppy*)$_3$	1.1 (7.3mg in 10 mL H_2O)
furfuryl alcohol	different concentrations

furfuryl alcohol (mM)	5.039	10.036	15.038	20.034	25.036	30.038
I^0/I^{-1}	5.110	9.70	12.389	15.020	19.0	22.870
I^0/I^{-1}	5.129	9.874	12.663	15.954	20.967	24.032
I^0/I^{-1} average	5.119	9.787	12.526	15.487	19.983	23.451

4.11 Cyclic voltammetry (CV) experiments

Cyclic voltammograms were conducted on a Metrohm PGSTAT302N potentiostat and performed in a three-electrode cell connected to a Schlenk line under nitrogen at room temperature. The working electrode was a carbon plate electrode. The counter electrode was a platinum wire. The reference was a Hg/Hg_2Cl_2 electrode submerged in saturated aqueous KBr solution and separated from the reaction by a salt bridge.

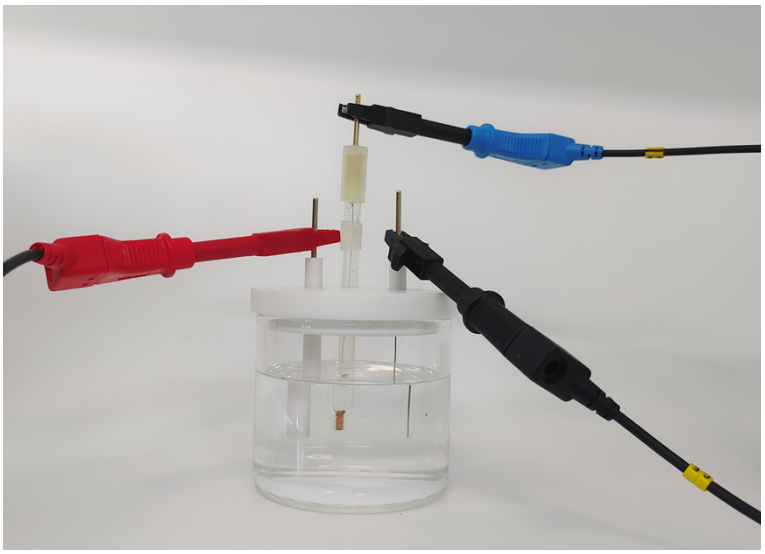


Figure S6. Cyclic voltammograms experiments

(A) CV Procedure for [Ir]. A solvent (H_2O, 40 mL) containing tris (2-phenylpyridine) iridium ($Ir(ppy)_3$) (10.0 mg, 3.8×10^{-4} mol·L^{-1}, 3×10^{-3} chemical equivalent), was added to the electrochemical cell in cyclic voltammetry experiments. A constant current of 0.01 mA. The scan rate was 0.10 V/s, ranging from -3.0 V to 2.0 V.

(B) CV Procedure for FAL. A solvent (H_2O, 40 mL) containing FAL (80.0 mg, 0.02 mol·L^{-1}, 1 chemical equivalent), was added to the electrochemical cell in cyclic voltammetry experiments. A constant current of 0.01 mA. The scan rate was 0.10 V/s, ranging from -0.8 V to 1.5 V.

(C) CV Procedure for different gas without [Ir]. A solvent (H_2O, 40 mL) containing FAL (80.0 mg, 0.02 mol·L^{-1}, 1 chemical equivalent), O_2, or Ar are passed through respectively, was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 0.01 mA. The scan rate was 0.10 V/s, ranging from -0.8 V to 1.40 V.

(D) CV Procedure for different gas with [Ir]. A solvent (H_2O, 40 mL) containing FAL (80.0 mg, 0.02 mol·L^{-1}, 1 chemical equivalent), Tris (2-phenylpyridine) iridium (Ir (ppy)$_3$) (10.0 mg, 3.8×10^{-4} mol·L^{-1}, 3×10^{-3} chemical equivalent), O_2 and Ar are passed through respectively, was added into the electrochemical cell in cyclic voltammetry experiments. A constant current of 0.01 mA. The scan rate was 0.10 V/s, ranging from -3 V to 2.5 V.

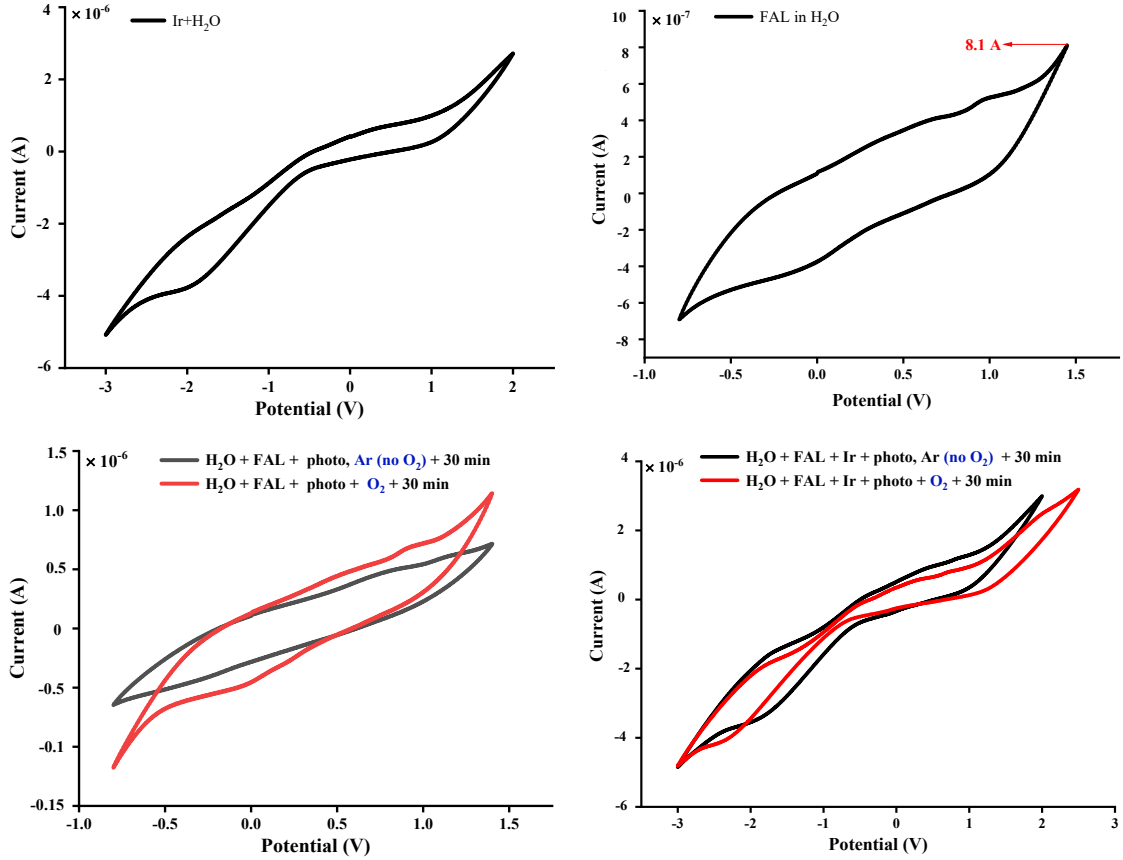


Figure S7. Cyclic voltammograms spectroscopies

4.12 Micro-Coulometric experiments

CV experiments for oxidation peak of A:

Using H_2O (40 mL) as a solvent in standard conditions, we performed cyclic voltammetry (CVs) experiments of reactant FAL (**A**, 80.0 mg) at a scan rate of 0.010 V/s, from – 3.0 V to 3.0 V.

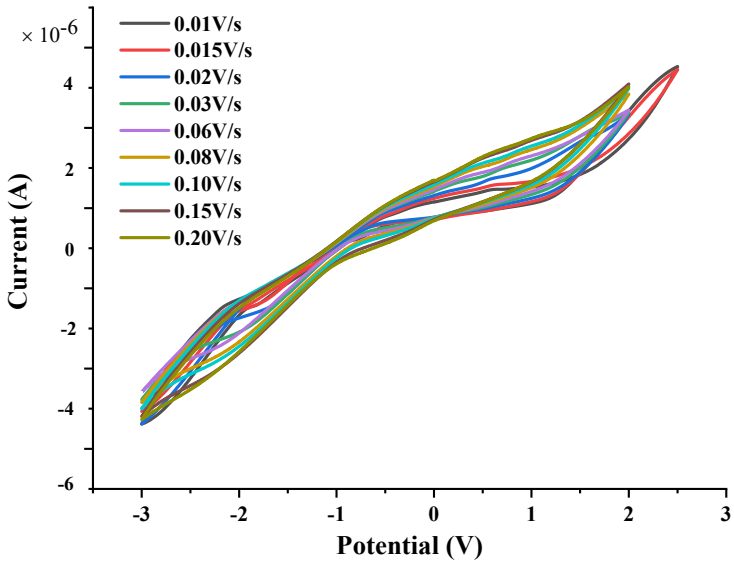


Figure S8. CVs of furfural alcohol at different scan rates

E_{pa1}	I_{pa1}	$\log I_{pa1}$
0.609	$4.650*10^{-7}$	-6.333
0.631	$5.820*10^{-7}$	-6.235
0.596	$7.390*10^{-7}$	-6.131
0.694	$9.850*10^{-7}$	-6.007
0.834	$1.180*10^{-6}$	-5.928
0.879	$1.365*10^{-6}$	-5.865
0.932	$1.493*10^{-6}$	-5.826
0.961	$1.655*10^{-6}$	-5.781
1.008	$1.745*10^{-6}$	-5.758

CV experiments for oxidation peak of Ferrocene:

Using H_2O (40 mL) as a solvent, we performed cyclic voltammetry (CVs) experiments of Ferrocene (74.4 mg) were conducted at a scan rate of 0.010 V/s, from -0.5 V to 0.9 V.

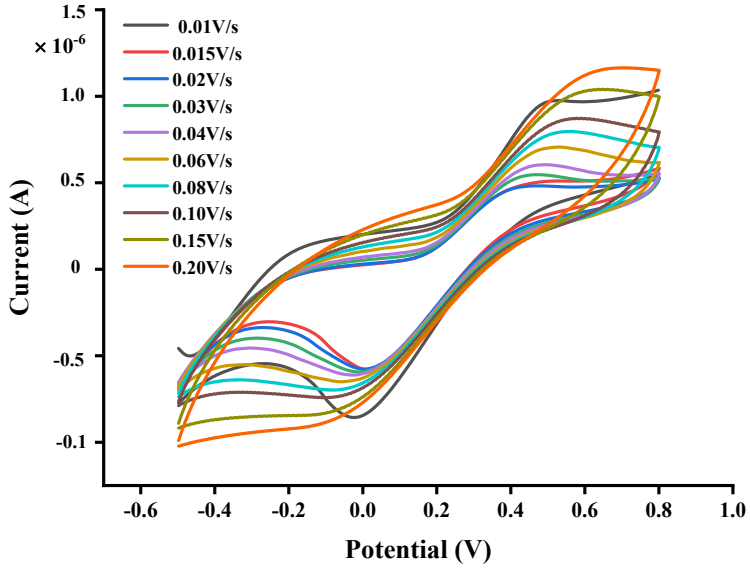


Figure S9. CVs of Ferrocene at different scan rates

E_{pa}	I_{pa}	$\log I_{pa}$
0.020	$-5.83*10^{-7}$	-6.234
0.003	$-5.76*10^{-7}$	-6.240
-0.011	$-5.93*10^{-7}$	-6.227
-0.028	$-6.11*10^{-7}$	-6.214
-0.05	$-6.49*10^{-7}$	-6.188
-0.07	$-6.97*10^{-7}$	-6.157
-0.09	$-7.41*10^{-7}$	-6.130
-0.11	$-8.34*10^{-7}$	-6.079
-0.13	$-9.04*10^{-7}$	-6.044

5. DFT calculations and mechanism

Geometries and Energies for All Optimized Starting Materials, Transition States, Intermediates, and Target Materials

Single Point Energy■,Δ (*E*M06, in Hartree)
Zero-point correction (*E*0, in Hartree)
Thermal correction to Enthalpy (*H*, in Hartree)
Thermal correction to Gibbs Free Energy (*G*, in Hartree)
Sum of electronic and zero-point Energies (*E*M06+*E*0, in Hartree)
Sum of electronic and thermal Enthalpies (*E*M06+*H*, in Hartree)
Sum of electronic and thermal Free Energies (*E*M06+*G*, in Hartree)
■ The single-point energies and solvent effects were computed at the M06/6-31+G(d) level
Δ The single-point energies and solvent effects were computed at the M06/6-311+G(2d,2p) level

Gaussian program 16 was employed for DFT calculations,[7] and /M06-2X/def2-SVP level were used for geometry optimization and frequency calculations. The 6-311+G(2d,p) basis sets were employed in the calculations of triplet-singlet energy gaps. In the model substrate's reaction profile calculations, 6-31G(d,p) basis sets were used. Optimizations were conducted without constraint using the implicit solvation model (SMD)19 in dichloromethane (ε = 8.93). Frequency analyses (at 298.15 K and 1 atm) were carried out to confirm that each structure is a minimum (no imaginary frequency) or a transition state (only one imaginary frequency). The searching for minimal energy crossing points was conducted using a modified version of Harvey's code20 (sobMECP21) interfaced with Gaussian 16. The Gibbs free energies in dichloromethane (ΔG) were discussed throughout this Article unless otherwise specified. The single-point calculations were at M06-2X/def2-TZVP level. The SMD implicit solvent model was used to account for water's solvation effect. The 3D images of the calculated structures and the orbital diagrams were prepared using CYLView22 or VMD.

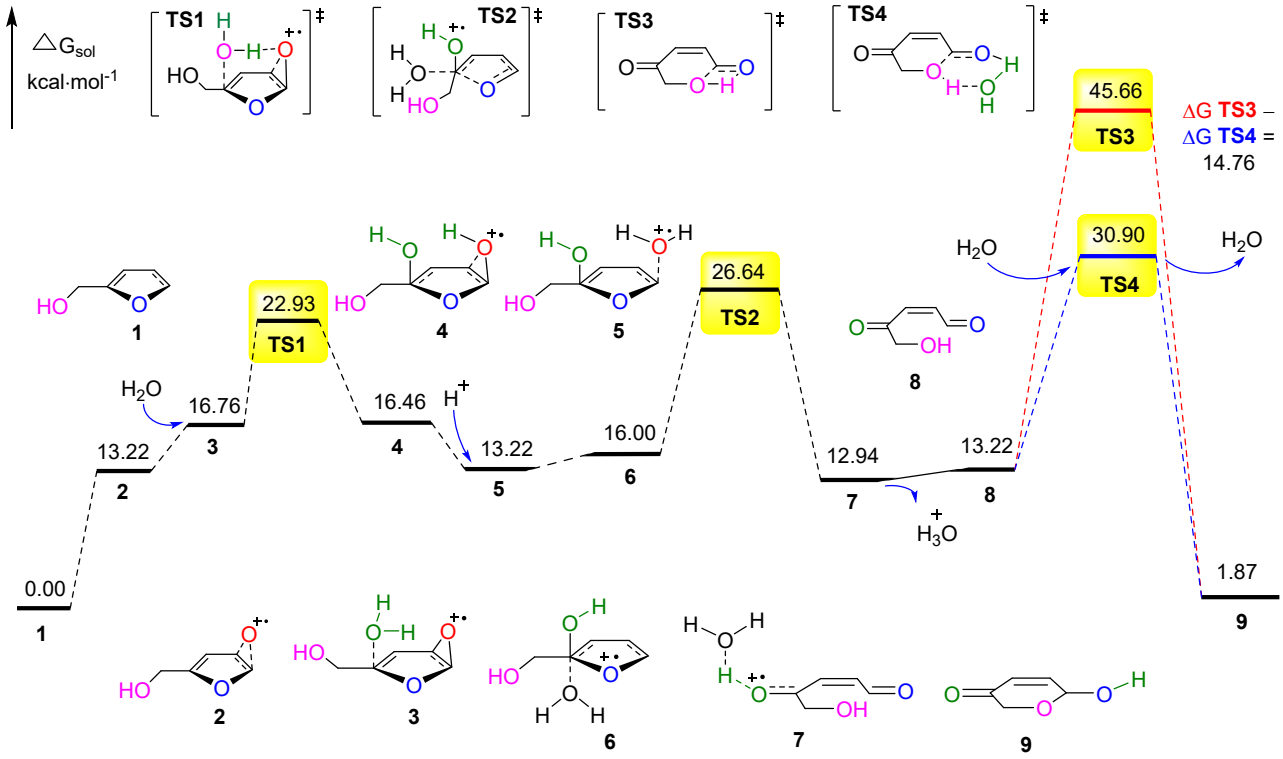
DFT calculation details (including reaction energy barriers and pathways, optimized structures with exact bond length and bond angle, and molecule electro-static potentials)

5.1 Route A: an oxygen onium ion oxidation

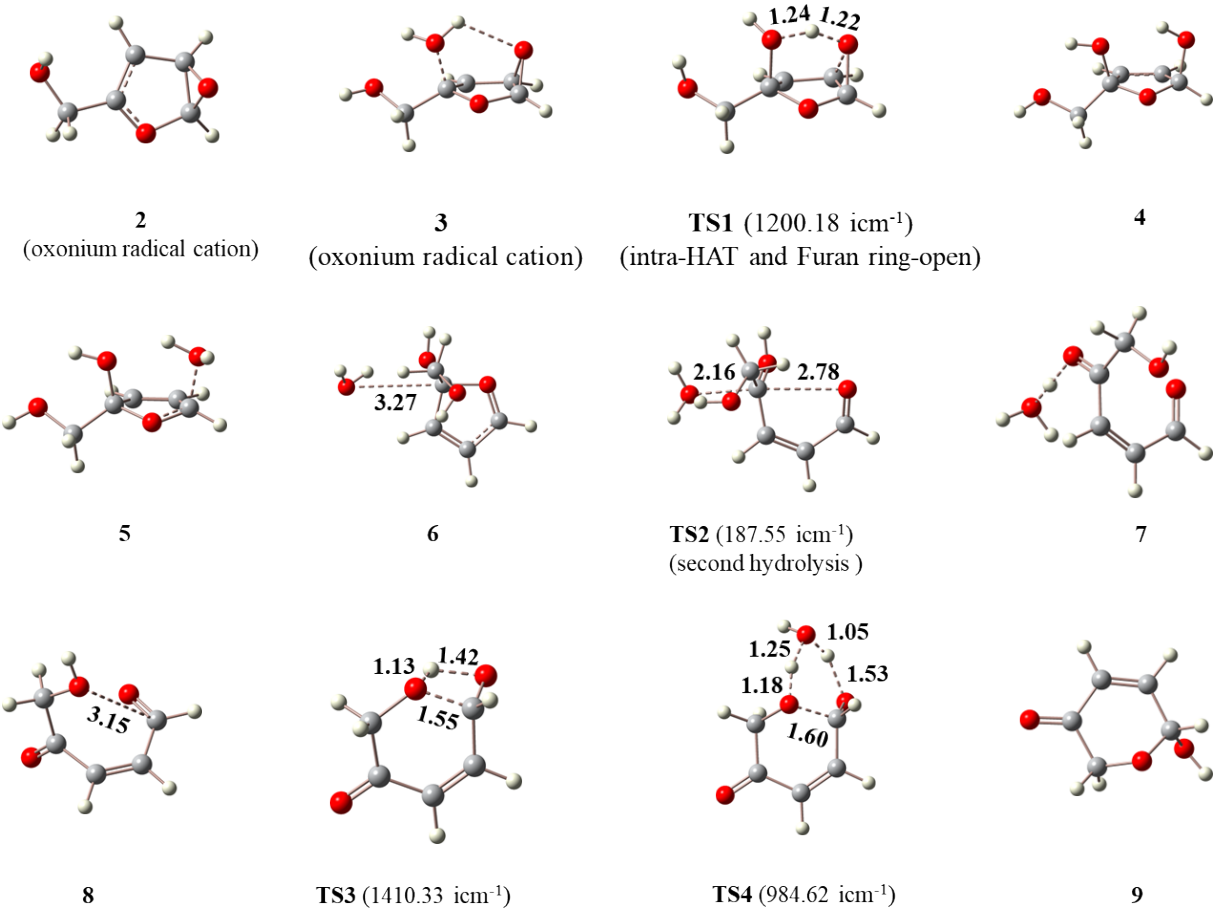
For the oxygen onium ion oxidation process, as depicted in ***Figure S10-A***, FAL **1** and a singlet oxygen originating from the visible light irradiation and oxygen atmosphere could be transferred to form the essential oxygen cation radical **2**. Following the oxygen transfer, the epoxidated furan **3** can attract an H_2O of hydrolysis process to form a hydroxylation product **4**, with a hydrogen atom transformation to **5**, (bond distance **a** and **b** of optimized structure C4--H_2O--$O^{+\bullet}$ for **3** was demonstrated in PES, depicted in ***Figure S10-B***), this HAT process needs to bridge the hydrogen bond distance of **c** 1.22 Å, and **d** 1.24 Å of **TS1** with the first energy barrier of $\triangle G_{sol}$ = 22.93 kcal mol^{-1} and could undergo smoothly. The second transition involves a further step of the hydrolysis process (bond distance **e** 2.16 Å) of **6** and induces the furan ring-opening process (bond distance **f** 2.78 Å), passing a **TS2** state through forming **7**, which involves the second energy barrier of $\triangle G_{sol}$ = 26.64 kcal mol^{-1}. After a dehydration process of **7** to form the stable intermediate **8**, the transformation facing the third energy bridge to reach the final pyranone product **9**, directly intramolecular semi-acetal formation process (bonds distance of **g** 1.55 Å and **h** 1.42 Å) needs to overcome the third high energy barrier obstacle of **TS3** $\triangle G_{sol}$ = 45.66 kcal mol^{-1}, which was hard to access. By taking advantage of the water solvent catalysis, with an intra-semi-acetal bond distance of **i** 1.60 Å similar to **g** of **TS3**, the third energy barrier could shrink to a **TS4** state $\triangle G_{sol}$ = 30.90 kcal mol^{-1} (with a similar bond distance of **i** 1.60 Å), which could make the entire transformation possible, and the third energy barrier finally raised to be the rate-determining step of the onium ion transformation.

ESP (Electro-Static Potentials) on vdW (Van Der Waals) surface was used to reveal the most susceptible reactive sites and reactivity of reactant and related intermediates (***Figure S10-C***). It might be expected that the singlet oxygen-induced oxygen onium ion unit was vulnerable nucleophilic to abstract hydrogen atom for HAT and led to the furan-ring opening. This could be seen from the onium ion of **TS1** with a 183.89 kcal mol^{-1}. The 181.19 kcal mol^{-1} of **TS4** also demonstrated a high reactivity in the water catalytic intra-semi-acetal HAT transformation process.

(A) Reaction energy barriers and pathways



(B) Potential Energy Surface



2 (oxonium radical cation)

3 (oxonium radical cation)

TS1 (1200.18 icm^{-1}) (intra-HAT and Furan ring-open)

4

5

6

TS2 (187.55 icm^{-1}) (second hydrolysis)

7

8

TS3 (1410.33 icm^{-1})

TS4 (984.62 icm^{-1}) (H_2O catalysis of intra-semi-acetal)

9

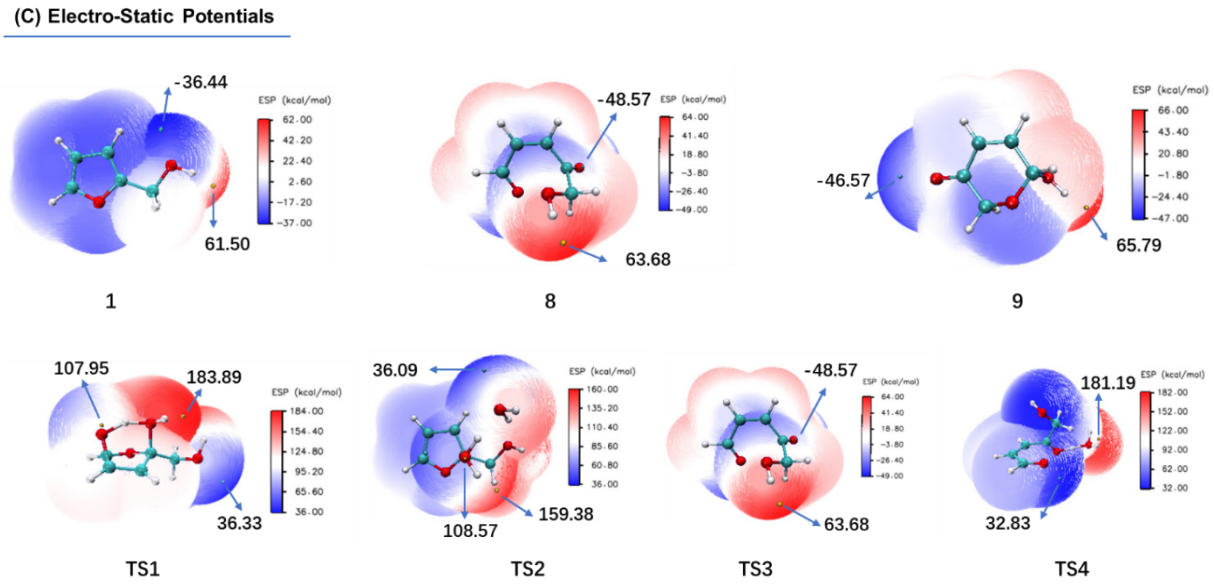


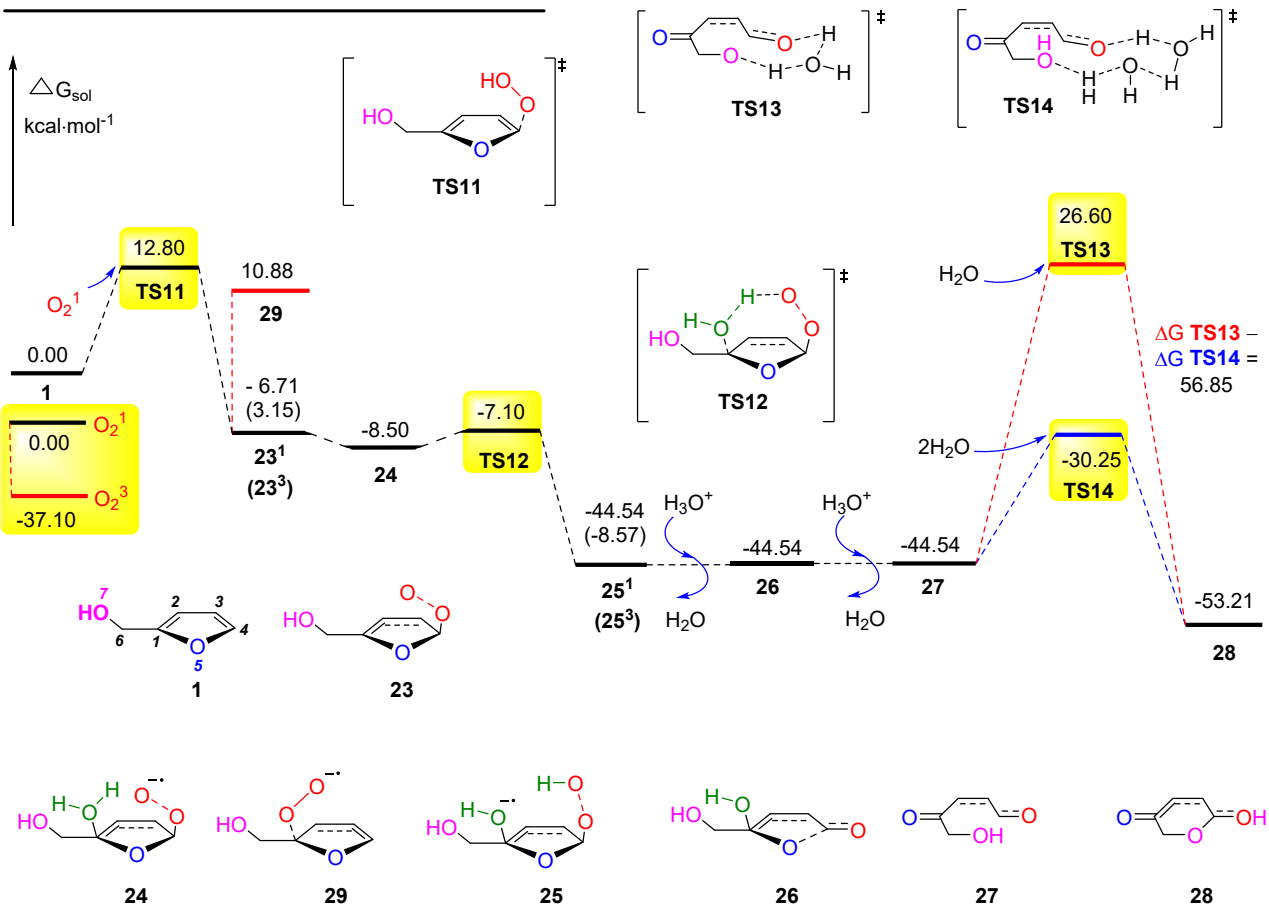
Figure S10. **An oxygen onium ion oxidation process. (A)** DFT-computed free energy surface and energy barriers for converting FAL into pyranone at the M062X(D3)/6-31G(d) level with the SMD solvation model and H_2O as the solvent. **(B)** Optimized corresponding structures of intermediates and transition states of PES (distances in Å). **(C)** ESP mapped molecular vdW surface of FAL, reaction intermediates, and area percent in each ESP range. Significant surface local minima and maxima of ESP are represented as orange and cyan spheres and labeled by dark blue and brown-red texts, respectively. The unit is in kcal mol^{-1}. Only the global minima and maxima on the surface are labeled. ESP calculated by Multiwfn 3.8 and visualized by the Visual Molecular Dynamics (VMD 1.9.3).

5.2 Route B: an endoperoxide-furan oxidation

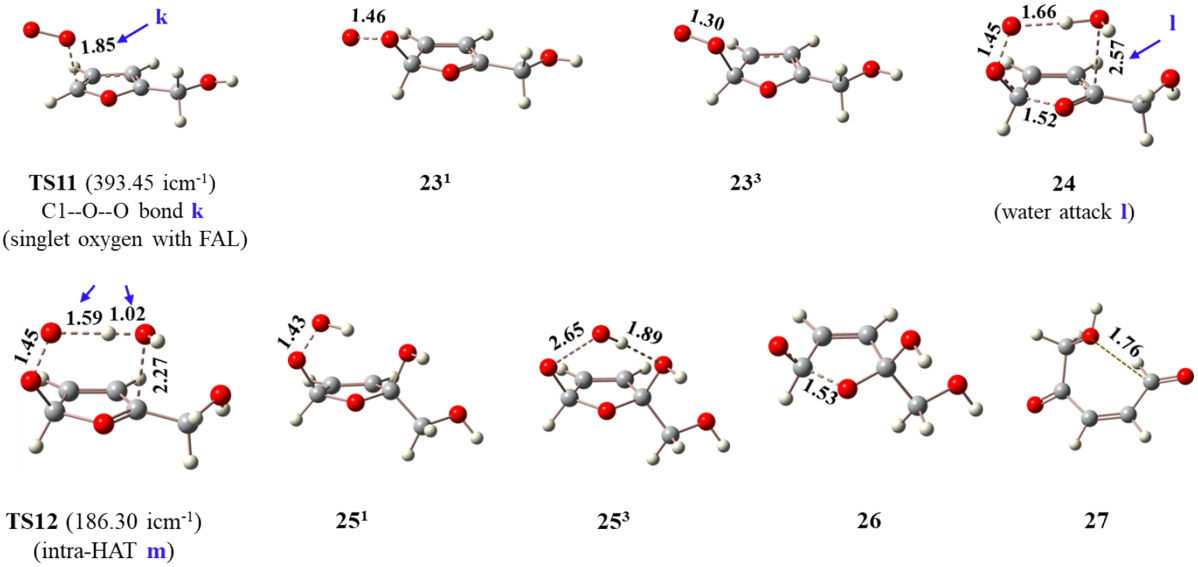
For the endoperoxide-furan process of photocatalytic singlet oxygen-induced oxidative reaction, as demonstrated in ***Figure S11-A***, DFT calculation has firstly proved that only two types of oxygen with singlet and triplet (doublet and quartet were excluded) could be involved in the FAL oxidation with an energy gap of 37.10 kcal mol^{-1}, under this reaction conditions, which suggested singlet oxygen to be the best oxidative media, after a transient intermediate of **TS11** (bond distance **k** 1.85 Å of optimized structure C1--O--O was demonstrated in PES, depicted in ***Figure S11-B***), the resulting singlet product $\mathbf{23^1}$ was also more stable than triplet product $\mathbf{23^3}$, at the same time, it was easier for the singlet oxygen to react with furan C1-site to form product **23** than C4-site product **29**, so the product of **23** was the optimized compound in next steps. Then, the first hydrolyzed product **24** (bond distance **l** 2.57 Å), underwent an intramolecular hydrogen atom transformation (HAT) process **TS12** (bonds distance of **m** 1.59 Å and 1.02 Å), and following twice hydrolysis processes and access the furan ring-open movement to stable product **27**, the next transformation facing the third energy bridge to reach the final pyranone product **28**, direct intramolecular semi-acetal formation process needs to overcome a high energy barrier obstacle of **TS13** $\triangle G_{sol}$ = 26.60 kcal mol^{-1} (**n** in PES), which could be decreased by a specific two molecules of water catalysis with a **TS14** state $\triangle G_{sol}$ = -30.25 kcal mol^{-1} (hydrogen bond distances were demonstrated as **o** in PES).

ESP on vdW surface (***Figure S11-C***) also demonstrated that the endoperoxide-furan intermediate **TS11** possessed a reasonable 74.5 kcal mol^{-1}, and **TS14** had a 97.08 kcal mol^{-1} of high reactivity in the specific two catalytic intra-semi-acetal transformation processes.

(A) Reaction energy barriers and pathways



(B) Potential Energy Surface



TS11 (393.45 icm^{-1})
C1--O--O bond **k**
(singlet oxygen with FAL)

23^1

23^3

24
(water attack **l**)

TS12 (186.30 icm^{-1})
(intra-HAT **m**)

25^1

25^3

26

27

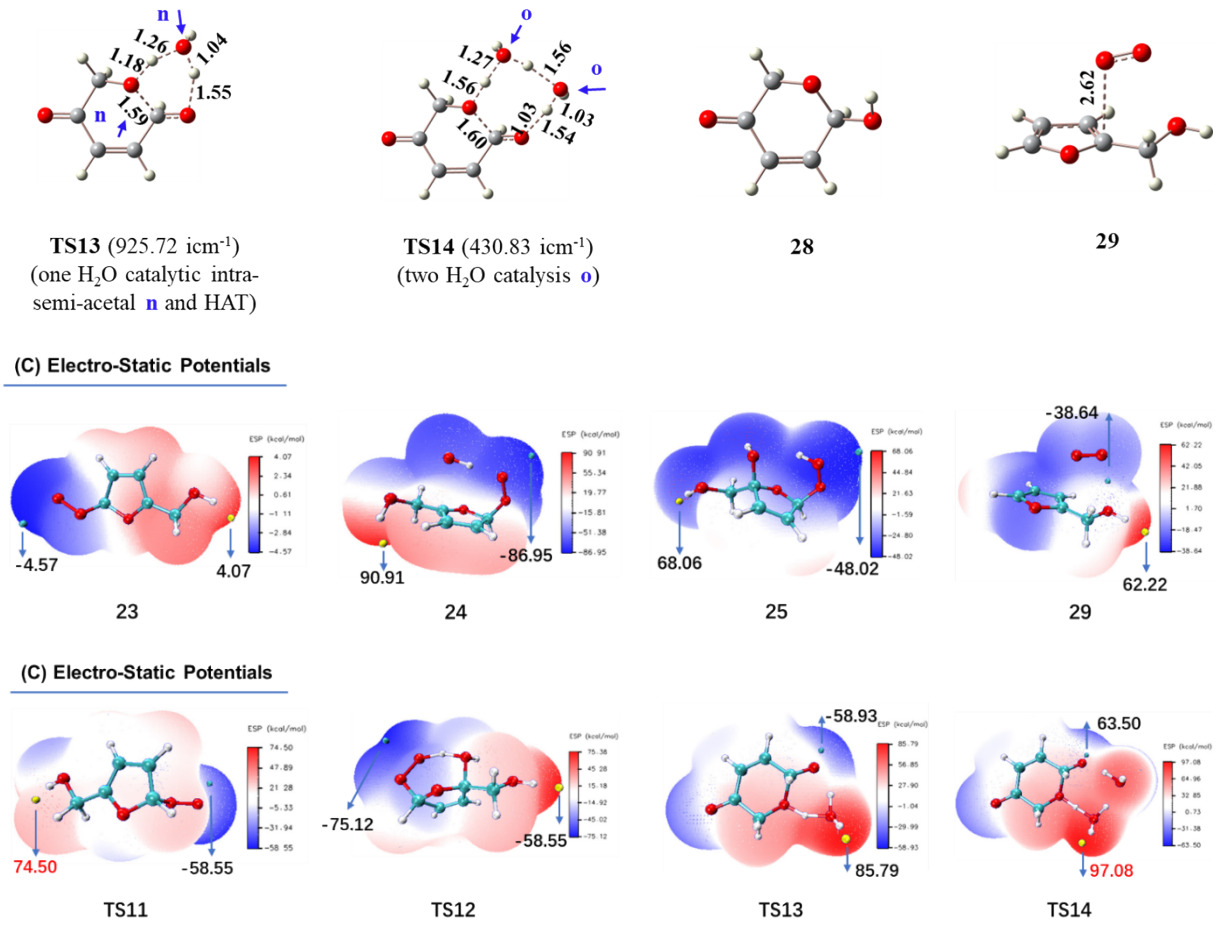


Figure S11. **An endoperoxide-furan process. (A)** DFT-computed free energy surface and energy barriers for converting FAL into pyranone at the M062X(D3)/6-31G(d) level with the SMD solvation model and H_2O as the solvent. **(B)** Optimized corresponding structures of intermediates and transition states of PES (distances in Å). **(C)** ESP mapped molecular vdW surface of FAL, reaction intermediates, and area percent in each ESP range. Significant surface local minima and maxima of ESP are represented as orange and cyan spheres and labeled by dark blue and brown-red texts. The unit is in kcal mol^{-1}. Only the global minima and maxima on the surface are labeled. ESP was calculated by Multiwfn 3.8 and further visualized by the Visual Molecular Dynamics (VMD 1.9.3).

5.3 DFT calculations original data

Standard orientation, imaginary frequencies, thermodynamic energies and single-point energies of All Stationary Points.

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.996664	-0.466731	-0.000090
2	6	0	-1.815284	0.874554	-0.000005
3	6	0	-0.392460	1.090816	-0.000101
4	6	0	0.176211	-0.140345	0.000036
5	8	0	-0.786476	-1.106695	0.000130
6	1	0	-2.865556	-1.107278	-0.000130
7	1	0	-2.591581	1.626317	-0.000015
8	1	0	0.129757	2.036384	-0.000178
9	6	0	1.587766	-0.621256	0.000113
10	1	0	1.763736	-1.248101	0.885250
11	1	0	1.763715	-1.248428	-0.884796
12	8	0	2.424261	0.521024	-0.000106
13	1	0	3.340226	0.204245	-0.000039

0 imaginary frequencies

Zero-point Energies = -344.305620

Thermal Energies = -344.300013

Thermal Enthalpies = -344.299068

Thermal Free Energies = -344.335112

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.715151	-0.572940	-0.264185
2	6	0	1.527543	0.881242	-0.327181
3	6	0	0.073970	1.060611	-0.245568
4	6	0	-0.490319	-0.241228	-0.107071
5	8	0	0.406578	-1.179887	-0.155511
6	1	0	2.441957	-1.225724	-0.729856
7	1	0	2.207906	1.588152	-0.782086
8	1	0	-0.495544	1.976617	-0.314621
9	6	0	-1.919503	-0.609531	0.067081
10	1	0	-2.186532	-1.271446	-0.765745
11	1	0	-2.005831	-1.196184	0.991467
12	8	0	-2.750290	0.520645	0.038690
13	1	0	-2.740198	0.928913	0.919790
14	8	0	2.010861	0.170586	0.859645

0 imaginary frequencies

Zero-point Energies = -419.240295

Thermal Energies = -419.233401

Thermal Enthalpies = -419.232457

Thermal Free Energies = -419.272206

3

Standard orientation:

Atomic Number	Atomic Number	Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.790663	-0.482839	-0.536726
2	6	0	1.680473	0.957105	-0.274505
3	6	0	0.247697	1.205669	-0.185439
4	6	0	-0.401605	-0.130204	-0.157488
5	8	0	0.504177	-1.051500	-0.640911
6	1	0	2.541509	-1.021246	-1.100498

7	1	0	2.423157	1.698195	-0.536696
8	1	0	-0.278725	2.144330	-0.100746
9	6	0	-1.784858	-0.289997	-0.742498
10	1	0	-1.755095	0.051165	-1.782373
11	1	0	-2.058264	-1.348888	-0.709099
12	8	0	-2.627828	0.508191	0.067036
13	1	0	-3.534891	0.173298	-0.012946
14	8	0	2.090991	-0.028777	0.754925
15	8	0	-0.626175	-0.541315	1.330104
16	1	0	0.160937	-0.297101	1.875067
17	1	0	-1.422169	-0.050953	1.658001

Zero-point Energies = -495.617365

Thermal Energies = -495.608779

Thermal Enthalpies = -495.607834

Thermal Free Energies = -495.650942

4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.738032	-0.077499	0.659602
2	6	0	1.452586	-1.215965	-0.258770
3	6	0	0.114337	-1.099653	-0.614948
4	6	0	-0.463777	0.108076	0.088250
5	8	0	0.512849	0.445252	1.059494
6	1	0	2.430190	-0.177505	1.488582
7	1	0	2.195653	-1.907881	-0.633370
8	1	0	-0.441276	-1.735933	-1.293825
9	6	0	-1.805760	-0.094291	0.762096
10	1	0	-1.764659	-0.976756	1.409908
11	1	0	-2.003478	0.796766	1.368427

12	8	0	-2.735539	-0.237492	-0.293150
13	1	0	-3.622690	-0.062056	0.057011
14	8	0	2.329875	0.654407	-0.414338
15	8	0	-0.512028	1.138630	-0.865092
16	1	0	1.643015	1.203488	-0.857629
17	1	0	-1.410512	1.129496	-1.251794

Zero-point Energies = -495.617179

Thermal Energies = -495.608175

Thermal Enthalpies = -495.607231

Thermal Free Energies = -495.651419

5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.644526	0.210893	0.607215
2	6	0	-1.234061	1.374631	-0.231473
3	6	0	0.024017	1.177025	-0.604214
4	6	0	0.533358	-0.129104	-0.042624
5	8	0	-0.531276	-0.560831	0.819591
6	1	0	-2.203430	0.385461	1.523691
7	1	0	-1.907150	2.184290	-0.479407
8	1	0	0.637727	1.800764	-1.242938
9	6	0	1.788176	-0.029077	0.810953
10	1	0	1.677103	0.788075	1.532154
11	1	0	1.905600	-0.976125	1.350103
12	8	0	2.857551	0.190121	-0.090973
13	1	0	3.685546	-0.024935	0.365347
14	8	0	-2.655724	-0.585832	-0.217684
15	8	0	0.703179	-1.082596	-1.055762
16	1	0	-2.233695	-0.950639	-1.031983

17	1	0	1.664332	-1.175246	-1.193704
18	1	0	-3.017659	-1.344753	0.296219

Zero-point Energies = -496.280044

Thermal Energies = -496.270738

Thermal Enthalpies = -496.269794

Thermal Free Energies = -496.314036

6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.104604	-0.609831	-0.067719
2	6	0	1.387433	-1.133992	1.056249
3	6	0	0.087564	-0.893152	0.803242
4	6	0	-0.039292	-0.096969	-0.452939
5	8	0	1.357295	-0.123279	-0.977943
6	1	0	3.177444	-0.586535	-0.237868
7	1	0	1.845787	-1.623211	1.903022
8	1	0	-0.781263	-1.132231	1.405915
9	6	0	-0.296343	1.407865	-0.169510
10	1	0	-0.306491	1.907486	-1.142883
11	1	0	-1.287214	1.471127	0.288509
12	8	0	0.718234	1.977883	0.612110
13	1	0	0.498117	1.855059	1.549535
14	8	0	-0.898784	-0.638590	-1.361950
15	1	0	-1.096351	0.014364	-2.060205
16	8	0	-3.110154	-0.444089	0.601385
17	1	0	-2.643610	-0.601697	-0.236163
18	1	0	-3.402946	0.476714	0.525396

Zero-point Energies = -496.273897

Thermal Energies = -496.263297

Thermal Enthalpies = -496.262352

Thermal Free Energies = -496.309581

7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.486594	0.205802	0.145393
2	6	0	1.570635	-0.296422	1.197778
3	6	0	0.264019	-0.543379	1.066040
4	6	0	-0.542754	-0.391468	-0.199039
5	8	0	2.123539	0.743776	-0.883353
6	1	0	3.559783	0.081668	0.362722
7	1	0	2.032781	-0.482827	2.162986
8	1	0	-0.297523	-0.884436	1.930862
9	6	0	-1.006140	1.030463	-0.493772
10	1	0	-0.126924	1.677017	-0.545990
11	1	0	-1.526537	1.024438	-1.456827
12	8	0	-1.873565	1.382646	0.571833
13	1	0	-2.507172	2.041971	0.246657
14	8	0	-0.073601	-0.979698	-1.323429
15	1	0	0.472691	-1.755846	-1.100245
16	8	0	-1.863048	-1.129803	0.160242
17	1	0	-2.451027	-0.434977	0.570489
18	1	0	-2.296784	-1.432351	-0.671400

Zero-point Energies = -496.266298

Thermal Energies = -496.256190

Thermal Enthalpies = -496.255245

Thermal Free Energies = -496.301541

8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.898033	0.291213	-0.336711
2	6	0	1.491808	-0.522041	0.826034
3	6	0	0.228405	-0.934337	0.960692
4	6	0	-0.865054	-0.667581	-0.031795
5	8	0	1.170444	0.477734	-1.297740
6	1	0	2.905951	0.734103	-0.305168
7	1	0	2.247047	-0.763231	1.566819
8	1	0	-0.069893	-1.543236	1.812063
9	6	0	-1.499073	0.705749	-0.103318
10	1	0	-1.563026	0.984008	-1.161821
11	1	0	-2.523715	0.587395	0.276497
12	8	0	-0.764629	1.638576	0.659948
13	1	0	-1.241131	2.482020	0.617791
14	8	0	-1.315808	-1.581195	-0.699158

Zero-point Energies = -419.484920

Thermal Energies = -419.476299

Thermal Enthalpies = -419.475355

Thermal Free Energies = -419.518661

9

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.921337	-0.275413	0.347434

2	6	0	1.513484	0.580032	-0.781741
3	6	0	0.244598	0.978711	-0.913143
4	6	0	-0.853029	0.688474	0.072417
5	8	0	1.117129	-0.764717	1.128089
6	1	0	2.998423	-0.467386	0.467259
7	1	0	2.278085	0.888007	-1.487064
8	1	0	-0.049535	1.618273	-1.743676
9	6	0	-1.599899	-0.630201	-0.008105
10	1	0	-1.861599	-0.923924	1.015068
11	1	0	-2.532015	-0.427851	-0.548404
12	8	0	-0.918434	-1.643002	-0.712614
13	1	0	-0.162893	-1.906464	-0.161303
14	8	0	-1.202371	1.553934	0.854144

Zero-point Energies = -419.487293

Thermal Energies = -419.478972

Thermal Enthalpies = -419.478028

Thermal Free Energies = -419.520493

H20

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000000	0.120386	0.000000
2	1	0	0.758741	-0.481532	-0.000000
3	1	0	-0.758741	-0.481553	-0.000000

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zero-point Energies = -76.366048

thermal Energies = -76.363213

thermal Enthalpies = -76.362269

thermal Free Energies = -76.384371

H30

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000090	-0.000090	-0.097230
2	1	0	0.687396	-0.608309	0.259265
3	1	0	-0.870490	-0.290432	0.259516
4	1	0	0.183812	0.899460	0.259061

zero-point Energies = -76.771602

thermal Energies = -76.768742

thermal Enthalpies = -76.767798

thermal Free Energies = -76.790744

O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.000000

zero-point Energies = -74.627936

thermal Energies = -74.626520

thermal Enthalpies = -74.625576

thermal Free Energies = -74.642506

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.724255	-0.669434	-0.339841
2	6	0	1.592553	0.739664	-0.722555
3	6	0	0.161159	0.974044	-0.789262
4	6	0	-0.444303	-0.180696	-0.051112
5	8	0	0.470742	-1.246073	-0.207191
6	1	0	2.531127	-1.358142	-0.549251
7	1	0	2.365796	1.333840	-1.188193
8	1	0	-0.357650	1.864710	-1.108866
9	6	0	-1.857572	-0.612319	-0.365502
10	1	0	-1.890575	-0.897202	-1.419501
11	1	0	-2.101265	-1.482334	0.252430
12	8	0	-2.750314	0.461841	-0.168332
13	1	0	-2.965676	0.506958	0.777127
14	8	0	1.974693	0.307205	0.715250
15	8	0	-0.295015	0.131903	1.395165
16	1	0	0.932658	0.326199	1.343124
17	1	0	-0.771807	0.959407	1.623630

Zero-point Energies = -495.608789

Thermal Energies = -495.601399

Thermal Enthalpies = -495.600454

Thermal Free Energies = -495.641107

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.550787	-0.040356	-0.171840
2	6	0	-1.575255	-0.677472	-1.092207

3	6	0	-0.257149	-0.694309	-0.877635
4	6	0	0.362822	-0.136295	0.346297
5	8	0	-2.232868	0.815974	0.631025
6	1	0	-3.596945	-0.367633	-0.268186
7	1	0	-1.972497	-1.122578	-1.999204
8	1	0	0.421082	-1.092654	-1.623957
9	6	0	1.054696	1.196242	0.312734
10	1	0	0.247300	1.920594	0.482515
11	1	0	1.760730	1.259623	1.148667
12	8	0	1.627721	1.470556	-0.936484
13	1	0	2.462804	0.978170	-0.992565
14	8	0	-0.001369	-0.657223	1.455049
15	1	0	0.361730	-0.187742	2.237903
16	8	0	2.186765	-1.266944	0.100491
17	1	0	2.598508	-1.270536	-0.781062
18	1	0	2.869328	-0.903001	0.691134

Zero-point Energies = -496.256834

Thermal Energies = -496.246512

Thermal Enthalpies = -496.245568

Thermal Free Energies = -496.292619

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.067554	0.774973	-0.548183
2	6	0	0.175823	1.903566	-0.133694
3	6	0	-0.988455	1.397535	0.249393
4	6	0	-0.971180	-0.105665	0.111205
5	8	0	0.290024	-0.381031	-0.498492
6	1	0	1.558672	0.859938	-1.516893

7	1	0	0.505789	2.934317	-0.133684
8	1	0	-1.851010	1.924403	0.639702
9	6	0	-2.048919	-0.675772	-0.799562
10	1	0	-2.065292	-0.113021	-1.739730
11	1	0	-1.799116	-1.722392	-1.008361
12	8	0	-3.269202	-0.566299	-0.088151
13	1	0	-3.916070	-1.153342	-0.508405
14	8	0	2.185828	0.669526	0.389412
15	8	0	-1.014049	-0.736895	1.366026
16	1	0	1.840149	0.601546	1.306098
17	1	0	-1.924903	-1.066159	1.478703
18	1	0	2.817306	-0.275466	0.185047
19	8	0	3.637258	-1.258181	-0.097506
20	1	0	3.330747	-2.000800	0.454835
21	1	0	3.455912	-1.573817	-1.002584

zero-point Energies = -419.435570

thermal Energies = -419.428858

thermal Enthalpies = -419.427914

thermal Free Energies = -419.466963

TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.152157	-0.451511	0.917486
2	6	0	-2.141166	-0.697181	-0.540161
3	6	0	-0.993264	-0.588619	-1.212480
4	6	0	0.297297	-0.208889	-0.575980
5	8	0	-1.118322	-0.348228	1.555476
6	1	0	-3.130946	-0.363379	1.411310
7	1	0	-3.068315	-0.965195	-1.034932

8	1	0	-0.932940	-0.788966	-2.280300
9	6	0	0.560940	1.226579	-0.164940
10	1	0	1.033892	1.208700	0.820964
11	1	0	1.298457	1.612977	-0.882912
12	8	0	-0.588688	2.030498	-0.095761
13	1	0	-0.834697	2.287744	-0.998338
14	8	0	1.201611	-1.048946	-0.523619
15	1	0	2.394208	-0.678405	0.011340
16	8	0	3.364389	-0.414573	0.452254
17	1	0	3.204693	-0.082257	1.359717
18	1	0	3.733826	0.336491	-0.057195

Zero-point Energies = -496.278105

Thermal Energies = -496.267625

Thermal Enthalpies = -496.266681

Thermal Free Energies = -496.314431

TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.529759	0.139606	-0.368382
2	6	0	0.630154	1.334782	-0.298467
3	6	0	-0.680302	1.312079	-0.036646
4	6	0	-1.432095	0.056415	0.067813
5	8	0	2.272238	-0.050607	0.738338
6	1	0	2.028515	0.029887	-1.338966
7	1	0	1.155282	2.281784	-0.402401
8	1	0	-1.253214	2.225697	0.090521
9	6	0	-0.725856	-1.239632	-0.262352
10	1	0	-1.041364	-2.027291	0.421999
11	1	0	-0.983745	-1.524305	-1.286222

12	8	0	0.709104	-1.164523	-0.185970
13	1	0	1.292278	-1.072199	0.776401
14	8	0	-2.622306	0.023497	0.338490

Zero-point Energies = -419.435570

Thermal Energies = -419.428858

Thermal Enthalpies = -419.427914

Thermal Free Energies = -419.466963

TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.823931	1.025672	0.266058
2	6	0	0.533506	1.674729	0.196652
3	6	0	1.686268	1.012066	0.058448
4	6	0	1.707906	-0.452159	-0.069589
5	8	0	-1.473306	0.980937	-0.876093
6	1	0	-1.385659	1.382815	1.144545
7	1	0	0.518925	2.761893	0.216929
8	1	0	2.641706	1.522382	-0.017763
9	6	0	0.376711	-1.169155	-0.019243
10	1	0	-0.011760	-1.249908	-1.042864
11	1	0	0.503161	-2.167362	0.401739
12	8	0	-0.552091	-0.452795	0.803411
13	1	0	-1.626686	-0.893682	0.572835
14	8	0	2.732960	-1.079703	-0.286686
15	8	0	-2.745753	-0.957724	0.018640
16	1	0	-2.727179	-1.713711	-0.595900
17	1	0	-2.489746	-0.115073	-0.547656

Zero-point Energies = -495.841663

Thermal Energies = -495.833302

Thermal Enthalpies = -495.832358

Thermal Free Energies = -495.874857

10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.231728	1.885687	-0.527746
2	6	0	-1.385740	1.677337	0.832694
3	6	0	-0.900888	0.419628	1.131497
4	6	0	-0.406830	-0.206833	-0.143005
5	8	0	-0.660182	0.808196	-1.145537
6	1	0	-1.472627	2.725844	-1.162574
7	1	0	-1.815251	2.395417	1.518630
8	1	0	-0.876359	-0.085365	2.086685
9	6	0	-1.171301	-1.452422	-0.572750
10	1	0	-2.229314	-1.184619	-0.672942
11	1	0	-0.790006	-1.774142	-1.551034
12	8	0	-0.970377	-2.441363	0.419969
13	1	0	-1.563950	-3.180622	0.218719
14	6	0	3.253445	0.016677	-0.031368
15	1	0	3.380061	-0.106249	-1.110601
16	1	0	3.472981	-0.937051	0.457050
17	1	0	3.973211	0.760157	0.321378
18	6	0	1.845812	0.466581	0.292466
19	1	0	1.715998	0.608009	1.371617
20	1	0	1.613592	1.414916	-0.207116
21	8	0	0.952440	-0.551361	-0.169500

Zero-point correction = 0.175617 (Hartree/Particle)

Thermal correction to Energy = 0.186139

Thermal correction to Enthalpy = 0.187083

Thermal correction to Gibbs Free Energy = 0.138924

Sum of electronic and zero-point Energies = -498.573842

Sum of electronic and thermal Energies = -498.563320

Sum of electronic and thermal Enthalpies = -498.562376

Sum of electronic and thermal Free Energies = -498.610535

11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.127237	-1.018841	0.630812
2	6	0	0.396438	-0.644150	1.892605
3	6	0	-0.593861	0.186520	1.599805
4	6	0	-0.647443	0.412994	0.104946
5	8	0	0.327264	-0.489133	-0.416193
6	1	0	1.231698	-2.096420	0.452785
7	1	0	0.717305	-0.984946	2.869452
8	1	0	-1.276668	0.678243	2.282539
9	6	0	-0.260849	1.826215	-0.305869
10	1	0	0.757595	2.011478	0.057116
11	1	0	-0.262433	1.877387	-1.403083
12	8	0	-1.196000	2.724540	0.262364
13	1	0	-0.881592	3.623985	0.084244
14	6	0	-3.628314	-1.361232	-1.067659
15	1	0	-3.267515	-1.426379	-2.097920
16	1	0	-4.365497	-0.555630	-1.005849
17	1	0	-4.121539	-2.302483	-0.810815
18	6	0	-2.479193	-1.103924	-0.118015
19	1	0	-2.830839	-1.056056	0.919722
20	1	0	-1.727413	-1.898826	-0.186931
21	8	0	-1.889986	0.147474	-0.482495

22	6	0	3.195010	0.320257	-1.513422
23	1	0	3.435357	1.299761	-1.088698
24	1	0	2.206180	0.372067	-1.975206
25	1	0	3.931205	0.094749	-2.291180
26	6	0	3.245484	-0.745134	-0.432504
27	1	0	2.967092	-1.728333	-0.831710
28	1	0	4.257510	-0.821509	-0.024613
29	8	0	2.396536	-0.423297	0.674569

Zero-point correction = 0.252061 (Hartree/Particle)

Thermal correction to Energy = 0.266293

Thermal correction to Enthalpy = 0.267237

Thermal correction to Gibbs Free Energy = 0.210446

Sum of electronic and zero-point Energies = -652.919973

Sum of electronic and thermal Energies = -652.905741

Sum of electronic and thermal Enthalpies = -652.904797

Sum of electronic and thermal Free Energies = -652.961588

12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.986363	-1.216593	0.486755
2	6	0	0.322758	-0.952464	1.799514
3	6	0	-0.608660	-0.027681	1.606490
4	6	0	-0.647062	0.379973	0.150813
5	8	0	0.292058	-0.536679	-0.471256
6	1	0	1.194237	-2.245831	0.193100
7	1	0	0.619924	-1.440878	2.718589
8	1	0	-1.261367	0.420640	2.345543
9	6	0	-0.157030	1.799554	-0.092600
10	1	0	0.868224	1.879485	0.288473

11	1	0	-0.152372	1.977904	-1.175746
12	8	0	-1.043258	2.670131	0.582869
13	1	0	-0.703224	3.571990	0.477365
14	6	0	-3.739100	-1.040077	-1.184714
15	1	0	-3.391689	-1.020031	-2.221179
16	1	0	-4.407640	-0.190244	-1.021487
17	1	0	-4.303906	-1.961951	-1.023585
18	6	0	-2.567705	-0.984366	-0.230828
19	1	0	-2.905342	-1.012333	0.811555
20	1	0	-1.882886	-1.823815	-0.395290
21	8	0	-1.877027	0.250460	-0.472763
22	6	0	3.087808	0.636107	-1.442006
23	1	0	3.388386	1.484165	-0.822177
24	1	0	2.072470	0.791565	-1.810862
25	1	0	3.765069	0.576352	-2.298990
26	6	0	3.203513	-0.652310	-0.672583
27	1	0	2.845865	-1.524756	-1.221549
28	1	0	4.209965	-0.833105	-0.299407
29	8	0	2.365987	-0.559207	0.559952
30	1	0	2.856894	-0.899662	1.340192

Zero-point correction = 0.264740 (Hartree/Particle)

Thermal correction to Energy = 0.279166

Thermal correction to Enthalpy = 0.280110

Thermal correction to Gibbs Free Energy = 0.223558

Sum of electronic and zero-point Energies = -653.320207

Sum of electronic and thermal Energies = -653.305780

Sum of electronic and thermal Enthalpies = -653.304836

Sum of electronic and thermal Free Energies = -653.361389

13

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.477646	-1.883993	-0.403819
2	6	0	0.531200	-1.701685	0.981242
3	6	0	0.707335	-0.348767	1.184682
4	6	0	0.760185	0.240614	-0.103141
5	8	0	0.603670	-0.701357	-1.045999
6	1	0	0.355060	-2.758370	-1.026786
7	1	0	0.445190	-2.488681	1.716354
8	1	0	0.794861	0.195920	2.114084
9	6	0	1.035732	1.634168	-0.531512
10	1	0	2.076099	1.672967	-0.882099
11	1	0	0.389095	1.873594	-1.380846
12	8	0	0.778628	2.542678	0.511177
13	1	0	1.548585	2.550067	1.101957
14	6	0	-3.976800	-0.145074	-0.153536
15	1	0	-4.121982	0.129726	-1.203432
16	1	0	-4.367264	0.660253	0.474989
17	1	0	-4.550698	-1.054788	0.045414
18	6	0	-2.505082	-0.375943	0.135989
19	1	0	-2.351075	-0.645675	1.184480
20	1	0	-2.120988	-1.199371	-0.483803
21	8	0	-1.734174	0.804436	-0.079177
22	1	0	-1.820047	1.039315	-1.018635
23	8	0	3.370440	-0.652628	-0.290087
24	1	0	3.837315	0.080297	-0.720063
25	1	0	3.556038	-0.516214	0.651639

Zero-point correction = 0.210709 (Hartree/Particle)

Thermal correction to Energy = 0.226326

Thermal correction to Enthalpy = 0.227270

Thermal correction to Gibbs Free Energy = 0.166687

Sum of electronic and zero-point Energies = -575.354329

Sum of electronic and thermal Energies = -575.338713

Sum of electronic and thermal Enthalpies = -575.337768

Sum of electronic and thermal Free Energies = -575.398351

14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.108719	-0.111945	-0.484561
2	6	0	-1.967802	0.185720	0.876050
3	6	0	-0.646995	0.533960	1.059950
4	6	0	-0.030711	0.428809	-0.211406
5	8	0	-0.931837	0.045735	-1.130113
6	1	0	-2.948347	-0.429397	-1.086283
7	1	0	-2.761026	0.139866	1.608085
8	1	0	-0.139276	0.828721	1.967192
9	6	0	1.335183	0.753960	-0.666442
10	1	0	1.589448	0.110934	-1.517999
11	1	0	1.320329	1.795302	-1.022515
12	8	0	2.197526	0.584266	0.435084
13	1	0	3.022124	1.059716	0.244437
14	8	0	0.932285	-1.953002	0.257625
15	1	0	1.120000	-2.204705	-0.660627
16	1	0	1.727232	-1.459447	0.525390

Zero-point correction = 0.127936 (Hartree/Particle)

Thermal correction to Energy = 0.137537

Thermal correction to Enthalpy = 0.138481

Thermal correction to Gibbs Free Energy = 0.092848

Sum of electronic and zero-point Energies = -420.465582

Sum of electronic and thermal Energies = -420.455981

Sum of electronic and thermal Enthalpies = -420.455037

Sum of electronic and thermal Free Energies = -420.500670

15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.386861	-1.749394	-0.527825
2	6	0	1.503925	-1.534037	0.882786
3	6	0	0.858963	-0.379820	1.135063
4	6	0	0.341266	0.215402	-0.145281
5	8	0	0.729689	-0.845983	-1.140619
6	1	0	1.788533	-2.564904	-1.123311
7	1	0	2.020889	-2.195361	1.562639
8	1	0	0.735252	0.124076	2.086646
9	6	0	1.129467	1.454446	-0.573042
10	1	0	2.191636	1.196331	-0.632013
11	1	0	0.763750	1.743860	-1.565379
12	8	0	0.863012	2.432106	0.407444
13	1	0	1.504797	3.149591	0.286566
14	6	0	-3.280031	-0.117041	-0.048760
15	1	0	-3.401466	-0.107077	-1.134942
16	1	0	-3.509101	0.876925	0.344309
17	1	0	-3.989298	-0.831889	0.375760
18	6	0	-1.875114	-0.522053	0.324307
19	1	0	-1.735013	-0.534225	1.410486
20	1	0	-1.618478	-1.505681	-0.082724
21	8	0	-0.985640	0.469295	-0.243266

Zero-point correction = 0.178649 (Hartree/Particle)

Thermal correction to Energy = 0.188935

Thermal correction to Enthalpy = 0.189879

Thermal correction to Gibbs Free Energy = 0.142972

Sum of electronic and zero-point Energies = -498.419432

Sum of electronic and thermal Energies = -498.409147

Sum of electronic and thermal Enthalpies = -498.408202

Sum of electronic and thermal Free Energies = -498.455109

16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.239161	2.551011	-0.031579
2	6	0	-0.335438	1.823392	1.122719
3	6	0	-0.615878	0.517125	1.178919
4	6	0	-0.448787	-0.492686	0.066370
5	8	0	0.485517	2.044218	-1.110860
6	1	0	0.441088	3.620108	0.142278
7	1	0	-0.532434	2.426081	2.004150
8	1	0	-1.039568	0.117461	2.095824
9	6	0	-1.498901	-0.387429	-1.036733
10	1	0	-1.463038	0.618873	-1.461209
11	1	0	-1.256298	-1.127495	-1.805255
12	8	0	-2.744023	-0.661654	-0.414102
13	1	0	-3.333116	-1.064029	-1.071913
14	6	0	3.090224	-1.178091	-0.327842
15	1	0	3.255597	-0.666478	-1.279860
16	1	0	2.913715	-2.239393	-0.520254
17	1	0	3.991589	-1.077305	0.281822
18	6	0	1.920722	-0.564296	0.402182
19	1	0	1.714404	-1.077262	1.346673
20	1	0	2.085276	0.498352	0.598218
21	8	0	0.769184	-0.699515	-0.466491
22	8	0	-0.835842	-1.829092	0.794748
23	1	0	-1.828621	-1.888145	0.706630
24	1	0	-0.453892	-2.586589	0.292317

Zero-point correction = 0.203835 (Hartree/Particle)

Thermal correction to Energy = 0.216823

Thermal correction to Enthalpy = 0.217767

Thermal correction to Gibbs Free Energy = 0.164601

Sum of electronic and zero-point Energies = -574.786269

Sum of electronic and thermal Energies = -574.773281

Sum of electronic and thermal Enthalpies = -574.772336

Sum of electronic and thermal Free Energies = -574.825502

Eth

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.180105	-0.203021	0.000004
2	1	0	1.283406	-0.832508	-0.888490
3	1	0	1.283496	-0.832411	0.888553
4	1	0	1.990849	0.531135	-0.000066
5	6	0	-0.166335	0.494782	0.000017
6	1	0	-0.292960	1.160008	0.872243
7	1	0	-0.293064	1.159577	-0.872549
8	8	0	-1.256794	-0.367046	0.000022

Zero-point correction = 0.065255 (Hartree/Particle)

Thermal correction to Energy = 0.069063

Thermal correction to Enthalpy = 0.070007

Thermal correction to Gibbs Free Energy = 0.039605

Sum of electronic and zero-point Energies = -154.225442

Sum of electronic and thermal Energies = -154.221634

Sum of electronic and thermal Enthalpies = -154.220690

Sum of electronic and thermal Free Energies = -154.251092

EtOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.221455	-0.220461	0.000008
2	1	0	-1.292655	-0.856086	0.887772
3	1	0	-1.292697	-0.855872	-0.887907
4	1	0	-2.068529	0.471080	0.000113
5	6	0	0.084053	0.546016	0.000069
6	1	0	0.145853	1.190972	-0.886030
7	1	0	0.145894	1.190761	0.886320
8	8	0	1.150657	-0.399307	-0.000068
9	1	0	1.981287	0.100270	-0.000186

Zero-point correction = 0.080912 (Hartree/Particle)

Thermal correction to Energy = 0.085237

Thermal correction to Enthalpy = 0.086182

Thermal correction to Gibbs Free Energy = 0.055467

Sum of electronic and zero-point Energies = -154.879013

Sum of electronic and thermal Energies = -154.874688

Sum of electronic and thermal Enthalpies = -154.873744

Sum of electronic and thermal Free Energies = -154.904458

TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.327059	-2.126666	-0.515630
2	6	0	0.560662	-2.015186	0.825111
3	6	0	0.985372	-0.682821	1.045049
4	6	0	0.938845	-0.044006	-0.186699

5	8	0	0.586814	-0.945669	-1.146709
6	1	0	-0.012986	-2.933379	-1.147913
7	1	0	0.432999	-2.797270	1.559481
8	1	0	1.261322	-0.216382	1.980224
9	6	0	1.600344	1.213556	-0.663060
10	1	0	2.558265	0.957911	-1.133333
11	1	0	0.968181	1.692533	-1.413211
12	8	0	1.775431	2.124392	0.402726
13	1	0	2.505189	1.796743	0.952221
14	6	0	-3.258485	0.756584	-0.082441
15	1	0	-3.234567	1.152416	-1.101293
16	1	0	-3.416365	1.586126	0.612075
17	1	0	-4.096905	0.059699	0.006871
18	6	0	-1.946322	0.034692	0.237394
19	1	0	-1.999579	-0.398816	1.248782
20	1	0	-1.828905	-0.797439	-0.477600
21	8	0	-0.909931	0.956395	0.113402

Zero-point correction = 0.174324 (Hartree/Particle)

Thermal correction to Energy = 0.184824

Thermal correction to Enthalpy = 0.185768

Thermal correction to Gibbs Free Energy = 0.137262

Sum of electronic and zero-point Energies = -498.531835

Sum of electronic and thermal Energies = -498.521335

Sum of electronic and thermal Enthalpies = -498.520391

Sum of electronic and thermal Free Energies = -498.568897

TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.633828	-1.473310	0.131290

2	6	0	0.414625	-1.039546	1.478416
3	6	0	-0.442902	-0.006463	1.397179
4	6	0	-0.767840	0.291118	-0.038485
5	8	0	-0.024926	-0.815100	-0.739265
6	1	0	1.262059	-2.283555	-0.229041
7	1	0	0.884957	-1.478057	2.346542
8	1	0	-0.836858	0.598678	2.205969
9	6	0	-0.104514	1.581349	-0.553383
10	1	0	0.978007	1.496923	-0.407769
11	1	0	-0.345713	1.644488	-1.617940
12	8	0	-0.671347	2.694290	0.098880
13	1	0	-0.150055	2.870300	0.898067
14	6	0	-4.224179	-0.723513	-0.551135
15	1	0	-4.101231	-0.901934	-1.622549
16	1	0	-4.695369	0.252031	-0.405198
17	1	0	-4.882882	-1.493646	-0.142063
18	6	0	-2.889078	-0.777162	0.150879
19	1	0	-2.991294	-0.597270	1.226371
20	1	0	-2.394322	-1.741991	-0.004496
21	8	0	-2.070903	0.271287	-0.416829
22	6	0	3.588168	-0.569656	-1.306735
23	1	0	4.056330	0.296230	-1.789821
24	1	0	2.577705	-0.667877	-1.725374
25	1	0	4.159930	-1.467024	-1.573826
26	6	0	3.521004	-0.340479	0.210794
27	1	0	3.112017	-1.290219	0.654030
28	1	0	4.579687	-0.336222	0.573131
29	8	0	2.818722	0.780162	0.569845

Zero-point correction = 0.247670 (Hartree/Particle)

Thermal correction to Energy = 0.262131

Thermal correction to Enthalpy = 0.263075

Thermal correction to Gibbs Free Energy = 0.206183

Sum of electronic and zero-point Energies = -652.811736

Sum of electronic and thermal Energies = -652.797275

Sum of electronic and thermal Enthalpies = -652.796331

Sum of electronic and thermal Free Energies = -652.853222

TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.476657	-0.215669	-0.174921
2	6	0	-1.925145	-0.988647	0.833954
3	6	0	-0.619644	-0.557271	1.000559
4	6	0	-0.397851	0.446471	-0.003771
5	8	0	-1.572548	0.693333	-0.638054
6	1	0	-3.453700	-0.187104	-0.633354
7	1	0	-2.443759	-1.762982	1.380230
8	1	0	0.130278	-0.902618	1.697637
9	6	0	0.536836	1.608508	0.081756
10	1	0	0.661356	2.053852	-0.911873
11	1	0	0.054753	2.346929	0.735266
12	8	0	1.751940	1.149115	0.632541
13	1	0	2.290551	1.921719	0.866100
14	8	0	0.433208	-0.602218	-1.374258
15	1	0	0.810780	0.019635	-2.025778
16	1	0	1.225019	-1.040843	-0.921250
17	8	0	2.426735	-1.495104	0.059272
18	1	0	3.220949	-1.571616	-0.494504
19	1	0	2.483868	-0.598326	0.446059

Zero-point correction = 0.154336 (Hartree/Particle)

Thermal correction to Energy = 0.164895

Thermal correction to Enthalpy = 0.165839

Thermal correction to Gibbs Free Energy = 0.118122

Sum of electronic and zero-point Energies = -496.838501

Sum of electronic and thermal Energies = -496.827942

Sum of electronic and thermal Enthalpies = -496.826998

Sum of electronic and thermal Free Energies = -496.874715

TS8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.310084	-1.357129	-0.282281
2	6	0	-2.139521	-0.308063	-1.301816
3	6	0	-1.015742	0.397298	-1.174019
4	6	0	-0.079829	0.097811	-0.060558
5	8	0	-1.396251	-1.559973	0.507338
6	1	0	-3.238641	-1.936310	-0.228259
7	1	0	-2.877207	-0.139856	-2.076089
8	1	0	-0.709436	1.198965	-1.839103
9	6	0	-0.259061	0.729694	1.301029
10	1	0	-0.010805	-0.003602	2.071493
11	1	0	0.470906	1.547397	1.358526
12	8	0	-1.577442	1.163028	1.506522
13	1	0	-1.694564	2.015017	1.055335
14	8	0	1.001586	-0.472792	-0.407323
15	8	0	1.207070	2.437586	-0.855072
16	1	0	0.780681	3.145213	-0.347083
17	1	0	1.991353	2.222683	-0.325878
18	6	0	2.076285	-0.711737	0.565296
19	1	0	2.346852	0.255895	0.993802
20	1	0	1.664907	-1.369721	1.334027
21	6	0	3.210923	-1.343711	-0.195571
22	1	0	3.571241	-0.673548	-0.979506
23	1	0	4.029939	-1.539931	0.500691
24	1	0	2.897231	-2.289974	-0.642149

Zero-point correction = 0.200394 (Hartree/Particle)

Thermal correction to Energy = 0.214319

Thermal correction to Enthalpy = 0.215264

Thermal correction to Gibbs Free Energy = 0.160184

Sum of electronic and zero-point Energies = -574.782223

Sum of electronic and thermal Energies = -574.768297

Sum of electronic and thermal Enthalpies = -574.767353

Sum of electronic and thermal Free Energies = -574.822433

TS9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.281228	-1.215031	-0.405800
2	6	0	-1.732937	-1.214767	0.970623
3	6	0	-0.502721	-0.826917	1.321043
4	6	0	0.609588	-0.383557	0.417096
5	8	0	-1.760105	-0.631206	-1.338727
6	1	0	-3.217483	-1.776466	-0.547439
7	1	0	-2.401376	-1.573427	1.747292
8	1	0	-0.213970	-0.869913	2.367547
9	6	0	1.075732	-1.383055	-0.650347
10	1	0	1.056660	-2.380179	-0.206253
11	1	0	0.403480	-1.342767	-1.505569
12	8	0	2.415907	-1.106155	-1.002670
13	1	0	2.425492	-0.341241	-1.603479
14	6	0	-0.309484	3.189878	-0.382138
15	1	0	-0.215977	3.115147	-1.468192
16	1	0	0.614464	3.601009	0.032595
17	1	0	-1.130212	3.872841	-0.148382
18	6	0	-0.617249	1.842515	0.219973

19	1	0	-0.677928	1.877522	1.310135
20	1	0	-1.519593	1.399180	-0.196451
21	8	0	0.501081	0.963825	-0.146515
22	8	0	1.764544	-0.013871	1.224142
23	1	0	2.560325	-0.381165	0.755054
24	1	0	1.494493	1.044316	0.630593

Zero-point correction = 0.201285 (Hartree/Particle)

Thermal correction to Energy = 0.213309

Thermal correction to Enthalpy = 0.214253

Thermal correction to Gibbs Free Energy = 0.163351

Sum of electronic and zero-point Energies = -574.752038

Sum of electronic and thermal Energies = -574.740015

Sum of electronic and thermal Enthalpies = -574.739070

Sum of electronic and thermal Free Energies = -574.789973

TS10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.476016	-1.141367	-0.435097
2	6	0	-2.092951	-1.013912	0.997418
3	6	0	-0.881753	-0.754747	1.510115
4	6	0	0.399274	-0.614628	0.786967
5	8	0	-1.718139	-1.024114	-1.378762
6	1	0	-3.543800	-1.350411	-0.602766
7	1	0	-2.923913	-1.101127	1.691458
8	1	0	-0.784014	-0.618600	2.584408
9	6	0	0.799310	-1.616002	-0.305643
10	1	0	1.649224	-2.163809	0.113971
11	1	0	-0.018597	-2.316469	-0.469014
12	8	0	1.233167	-1.026441	-1.507735

13	1	0	0.446095	-0.607946	-1.902475
14	6	0	-0.593107	3.350868	-0.435009
15	1	0	-0.978659	3.297360	-1.456402
16	1	0	0.463086	3.636537	-0.469534
17	1	0	-1.140980	4.126387	0.107109
18	6	0	-0.763548	2.022198	0.269982
19	1	0	-0.384549	2.063185	1.298352
20	1	0	-1.811228	1.717461	0.291622
21	8	0	-0.070596	0.981283	-0.444484
22	8	0	1.321634	-0.045837	1.471070
23	1	0	2.229532	-0.022048	0.938743
24	1	0	0.837561	1.293999	-0.622105
25	8	0	3.332740	0.055394	-0.030339
26	1	0	2.876997	-0.192743	-0.862101
27	1	0	3.945562	-0.678518	0.148324

Zero-point correction = 0.228250 (Hartree/Particle)

Thermal correction to Energy = 0.243195

Thermal correction to Enthalpy = 0.244140

Thermal correction to Gibbs Free Energy = 0.186243

Sum of electronic and zero-point Energies = -651.159116

Sum of electronic and thermal Energies = -651.144171

Sum of electronic and thermal Enthalpies = -651.143227

Sum of electronic and thermal Free Energies = -651.201123

6. NMR experiments

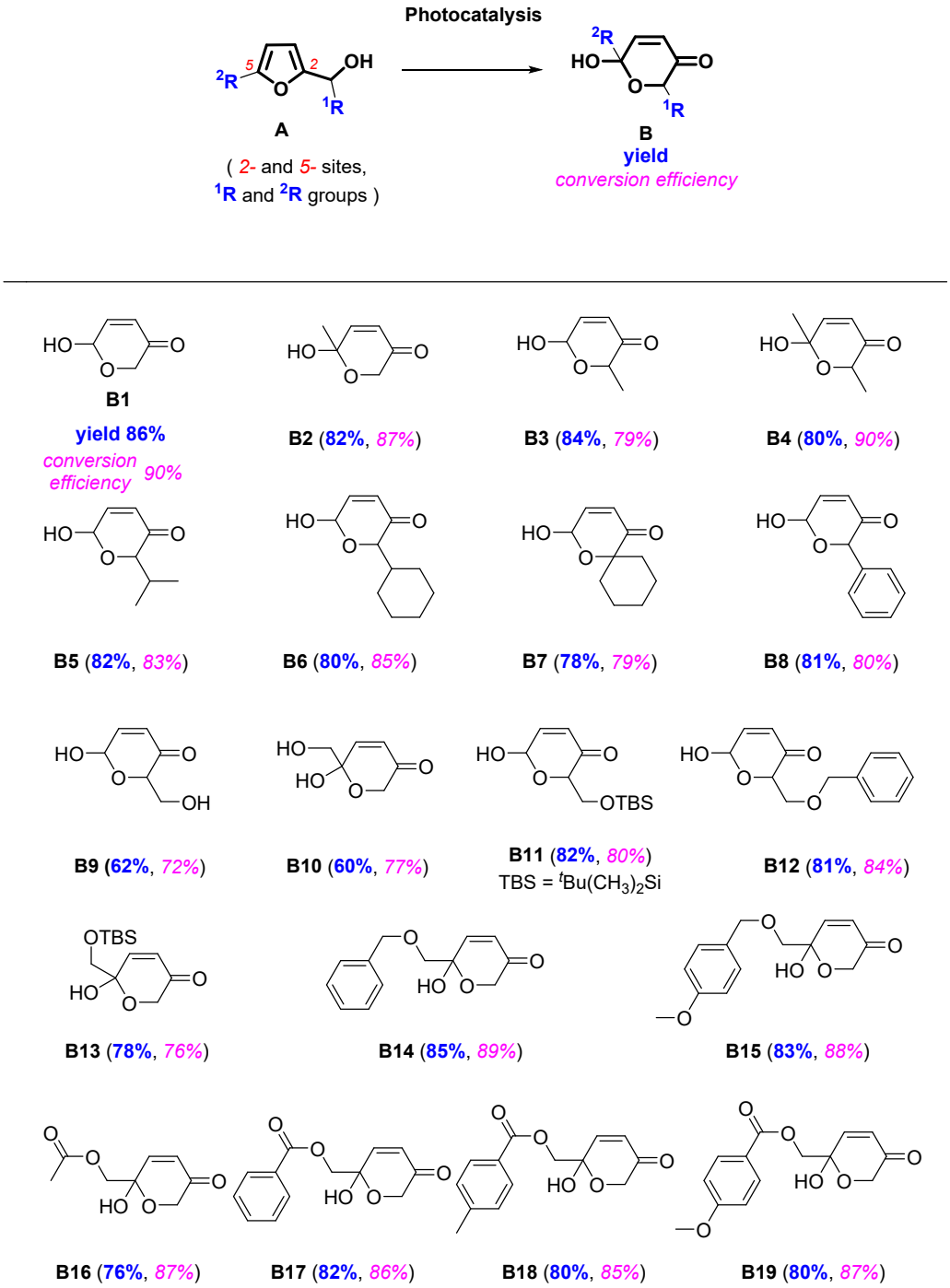


Figure S12. Chemical structures of the targeted products, including **yield**, and *conversion efficiency*.

6.1 Characterization of pyranone products

All the pyranone derivate products were produced according to the reaction process of *Supporting Information* **2.1 General photocatalysis**, and all spectral data of photocatalytic obtained pyranone products follow previous literature reported Achmatowicz rearrangement reaction pyranone products.[8-11]

B1: 6-hydroxy-2*H*-pyran-3(6*H*)-one. Yield 421.4 mg, 86%. Conversion efficiency 90%. Colorless oil. TLC: Petroleum ether/EtOAc = 5/1, R_f = 0.25. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 6.97–6.94 (m, 1H), 6.19–6.13 (m, 1H), 5.61–5.60 (d, J =2.6 Hz, 1H), 4.57–4.53 (d, J = 16.96 Hz, 1H), 4.25–4.24 (s, 1H), 4.14–4.09 (d, J = 16.96 Hz, 1H), 2.32–2.27 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 195.0, 146.2, 127.8, 88.2, 66.6. **HRMS (ESI$^+$):** calcd for $C_5H_7O_3$, $[M+Na]^+$ 115.0390, found 115.0387.

B2: 6-hydroxy-6-methyl-2*H*-pyran-3(6*H*)-one. Yield 381.3 mg, 82%. Conversion efficiency 87%. Yellow oil. TLC: Petroleum ether/EtOAc = 6/1, R_f = 0.5. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 6.87-6.85(d, J = 10.3Hz, 1H), 6.06-6.04 (d, J = 10.3Hz, 1H), 4.59-4.52 (d, J = 20.5Hz, 1H), 4.12-4.09 (d, J = 17Hz, 1H), 3.28-3.22 (d, J = 29.85Hz, 1H), 1.63 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 195.0, 149.1, 138.0, 132.4, 126.4, 92.8, 67.9, 66.5, 27.9. **HRMS (ESI$^+$):** calcd for $C_6H_9O_3$, $[M+H]^+$ 129.0546, found 129.0550.

B3: 6-hydroxy-2-methyl-2*H*-pyran-3(6*H*)-one. Yield 330.9 mg, 84%. Conversion efficiency 79%. Yellow oil. TLC: Petroleum ether/EtOAc = 7/1, R_f = 0.5. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 6.96-6.88 (m, 1H), 6.17-6.10 (q, J = 134.5Hz, 1H), 5.68-5.64 (d, J = 22.65Hz, 1H), 4.73-4.70 (q, J = 13.5Hz, 0.7H), 4.24-4.23 (q, J = 6.7Hz, 0.3H), 3.41 (s, 0.3H), 3.17 (s, 0.7H), 1.40-1.39 (d J = 6.75Hz, 2.5H), 1.26-1.23 (t, J = 13.85Hz, 0.5H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 196.8, 147.8, 144.2, 128.6, 127.3, 91.0, 87.8, 75.3, 70.4, 16.3, 15.3. **HRMS (ESI$^+$):** calcd for $C_6H_8NaO_3$, $[M+Na]^+$ 151.0366, found 151.0360.

B4: 6-hydroxy-2,6-dimethyl-2*H*-pyran-3(6*H*)-one. Yield 377.6 mg, 80%. Conversion efficiency 90%. Yellow oil. TLC: Petroleum ether/EtOAc = 6/1, R_f = 0.7. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 6.82-6.80 (d, J = 10.15Hz, 1H), 6.03-6.01 (d, J = 10.05Hz, 1H), 4.66-4.64 (q, J = 6.75Hz, 1H), 2.69 (s, 1H), 1.63-1.61 (s, 3H), 1.38-1.36 (d, J = 6.75Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 197.0, 147.8, 126.2, 92.9, 70.7, 29.0, 15.3. **HRMS (ESI$^+$):** calcd for $C_7H_{11}O_3$, $[M+H]^+$ 143.0703, found 143.0710.

B5: 6-hydroxy-2-isopropyl-2*H*-pyran-3(6*H*)-one. Yield 274.1 mg, 82%. Conversion efficiency

83%. Colorless oil. TLC: Petroleum ether/EtOAc = 5/1, R_f = 0.25. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.02–6.82 (m, 1H), 6.18–6.12 (m, 1H), 5.69–5.65 (m, 1H), 4.40–4.33 (d, *J* = 3.1 Hz, 0.75H), 3.90–3.80 (dd, *J* = 3.4, 1.4 Hz, 0.25H), 3.81–3.65 (m, 0.25H), 3.45 (d, *J* = 4.7 Hz, 0.75H), 2.58–2.30 (m, 1H), 1.05–1.00 (m, 3H), 0.93–0.81 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 195.8, 196.5, 149.5, 144.8, 129.7, 128.5, 94.1, 888.2, 82.3, 76.9, 29.5, 28.7, 18.9, 19.4, 16.4, 15.7. **HRMS (ESI$^+$):** calcd for $C_8H_{13}O_3$, $[M+H]^+$ 157.0859, found 157.0855.

B6: 2-cyclohexyl-6-hydroxy-2*H*-pyran-3(6*H*)-one. Yield 262.5 mg, 80%. Conversion efficiency 85%. Colorless oil. TLC: Petroleum ether/EtOAc = 5/1, R_f = 0.25. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 1.20-1.35 (m, 5H), 1.46 (s, 1H), 1.56-1.77 (m, 5H), 2.08-2.09 (d, 1H, *J* =2.7Hz), 3.87-3.88 (dd, 0.3H, *J* =1.55Hz), 4.36-4.37 (dd, 0.7H, *J* =1.75Hz), 5.61-5.65 (d, 1H, *J* =19.2Hz), 6.08-6.14 (m, 1H), 6.87-6.92 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 26.1, 26.14, 26.16, 26.4, 26.5, 26.6, 26.7, 29.3, 29.4, 38.5, 38.7, 78.5, 83.0, 87.6, 91.2, 128.2, 129.4, 144.3, 144.4, 147.9, 148.0, 196.1, 196.6, 196.7. **HRMS (ESI$^+$):** calcd for $C_{11}H_{17}O_3$ $[M+H]^+$ 197.1172; found 197.1180.

B7: 2-hydroxy-1-oxaspiro[5.5]undec-3-en-5-one. Yield 263.1 mg, 78%. Conversion efficiency 79%. Yellow oil. TLC: Petroleum ether/EtOAc = 3/1, R_f = 0.6. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 6.80 (dd, *J* = 10.3, 2.1 Hz, 1H), 6.00 (dd, *J* = 10.3, 1.4 Hz, 1H), 5.42 (t, *J* = 1.7 Hz, 1H), 1.90–1.49 (m, 9H), 1.35–1.00 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 197.9, 147.0, 125.8, 89.5, 82.3, 32.0, 31.0, 25.8, 21.0, 20.7. **HRMS (ESI$^+$):** calcd for $C_{10}H_{15}O_3$ $[M+H]^+$ 183.1016; found 183.1020.

B8: 6-hydroxy-2-phenyl-2*H*-pyran-3(6*H*)-one. Yield 265.3 mg, 81%. Conversion efficiency 80%. Colorless oil. TLC: Petroleum ether/EtOAc = 7/1, R_f = 0.30. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.38–7.21 (m, 5H), 6.79–6.56 (m, 1H), 6.21–6.10 (m, 1H), 5.60–5.57 (m, 1H), 5.53 (brs, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 197.0, 193.6, 147.7, 143.2, 134.5, 132.3, 128.4, 127.9, 127.5, 127.4, 127.3, 127.0, 126.0, 125.9, 91.5, 87.0, 80.1, 75.0. **HRMS (ESI$^+$):** calcd for $C_{11}H_{11}O_3$ $[M+H]^+$ 191.0703; found 191.0707.

B9: 6-hydroxy-2-(hydroxymethyl)-2*H*-pyran-3(6*H*)-one. Yield 328.0 mg, 62%. Conversion efficiency 72%. Colorless oil. TLC: Petroleum ether/EtOAc = 5/2, R_f = 0.30. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 3.86-3.89(m, 2H), 4.81-4.83(q, 1H, *J* =10.95Hz), 6.32-6.33(d, 1H, *J* =3.25Hz), 6.35-6.36(q, 1H, *J* =5.05Hz), 7.39-7.40(q, 1H, *J* =2.3Hz). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 65.1, 68.4, 107.1, 110.4, 142.4, 153.6. **HRMS (ESI$^+$):** calcd for $C_6H_9O_4$, $[M+H]^+$ 145.0495, found 145.0492.

B10: 6-hydroxy-6-(hydroxymethyl)-2*H*-pyran-3(6*H*)-one. Yield 301.0 mg, 60%. Conversion efficiency 77%. Colorless oil. TLC: Petroleum ether/EtOAc = 5/2, R_f = 0.35. **^{1}H NMR (**500 MHz, $CDCl_3$) δ ppm: 3.63-3.65 (d, 1H, *J* =11.4Hz), 3.80-3.82 (d, 1H, *J* =11.4Hz), 4.15-4.18 (d, 1H, *J* =16.9Hz), 4.59-4.63 (d, 1H, *J* =16.85Hz), 6.18-6.21 (d, 1H, *J* =10.4Hz), 6.82-6.84 (d, 1H, *J* =10.35Hz). **^{13}C NMR (**125 MHz, $CDCl_3$) δ ppm: 66.5, 67.6, 92.7, 128.9, 145.0, 194.5. **HRMS**

(ESI$^+$): calcd for $C_6H_9O_4$, $[M+H]^+$ 145.0495, found 145.0488.

B11: 2-(((*tert*-butyldimethylsilyl)oxy)methyl)-6-hydroxy-2*H*-pyran-3(6*H*)-one. Yield 271.9 mg, 82%. Conversion efficiency 80%. Yellow oil. TLC: Petroleum ether/EtOAc = 5/1, R_f = 0.6. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: δ 7.18 (dd, J = 12.0, 7.0 Hz, 1H), 6.19 (d, J = 12.0 Hz, 1H, 80%), 4.45 – 4.30 (m, 2H), 4.18 (dd, J = 13.5, 9.5 Hz, 1H), 4.08 (dd, J = 13.0, 5.5 Hz, 1H), 3.56 (br, 1H), 1.05 (s, 9H), 0.13 (s, 3H), 0.13 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 165.7, 143.8, 120.0, 78.7, 62.9, 62.3, 26.5, 17.3, -3.4. **HRMS (ESI$^+$):** calcd for $C_{12}H_{23}O_4Si$, $[M+H]^+$ 259.1360, found 259.1370.

B12: 2-((benzyloxy)methyl)-6-hydroxy-2*H*-pyran-3(6*H*)-one. Yield 260.8 mg, 81%. Conversion efficiency 84%. Yellow solid. TLC: Petroleum ether/EtOAc = 3/1, R_f = 0.55. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 7.36–7.21 (m, 5H), 6.87 (ddd, J = 16.4, 10.4, 3.3 Hz, 1H), 6.14 (ddd, J = 26.6, 10.3, 0.7 Hz, 1H), 5.62–5.39 (m, 1H), 4.66 (dd, J = 6.2, 2.7 Hz, 1H), 4.52 (d, J = 8.5 Hz, 2H), 3.92–3.74 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 196.2, 194.2, 148.3, 145.7, 137.2, 136.9, 128.5, 128.1, 128.0, 127.7, 127.7, 127.3, 127.1, 127.0, 87.4, 87.2, 77.5, 75.6, 75.0, 73.4, 71.0, 67.0. **HRMS (ESI$^+$):** calcd for $C_{13}H_{15}O_4$ $[M+H]^+$ 235.0965; found 235.0970.

B13: 6-(((*tert*-butyldimethylsilyl)oxy)methyl)-6-hydroxy-2*H*-pyran-3(6*H*)-one. Yield 284.7 mg, 78%. Conversion efficiency 76%. White solid. TLC: Petroleum ether/EtOAc = 3/1, R_f = 0.5. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm: 6.58 (d, 1H , J = 10.4 Hz), 6.20 (d, 1H, J = 10.4 Hz), 4.55 (d, 1H, J = 16.9 Hz), 4.10 (d, 1H, J = 16.9 Hz), 3.71 (q, 2H), 3.65 (br s, 1H), 0.96 (s, 9H), 0.10 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ ppm: 196.2, 145.2, 127.7, 92.0, 68.0, 66.9, 26.0, 18.5, −5.5, −5.9. **HRMS (ESI$^+$):** calcd for $C_{12}H_{23}O_4Si$, $[M+H]^+$ 259.1360, found 259.1365.

B14: 6-((benzyloxy)methyl)-6-hydroxy-2*H*-pyran-3(6*H*)-one. Yield 409.7 mg, 85%**.** Conversion efficiency 89%. Yellow oil**.** TLC: Petroleum ether/EtOAc = 8/1, R_f = 0.5. 1H NMR (500 MHz, CDCl3) δ ppm: 7.39-7.33 (m, 5H), 6.81-6.79 (d, J = 10.35Hz, 1H), 6.16-6.14 (d, J = 10.35Hz, 1H)**,** 4.73-4.71 (d, J = 12Hz, 1H), 4.66-4.59 (t, J = 32.35Hz, 2H), 4.19-4.15 (d, J = 17Hz, 1H), 3.73 (s, 1H), 3.66-3.64 (d, J = 10Hz, 1H), 3.58-3.57 (d, J = 7.96Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 194.8, 145.6, 037.0, 128.6, 128.5, 128.2, 128.0, 92.7, 74.1, 73.8, 66.6. **HRMS (ESI$^+$):** calcd for $C_{13}H_{15}O_4$, $[M+H]^+$ 235.0965, found 235.0967.

B15: 6-hydroxy-6-(((4-methoxybenzyl)oxy)methyl)-2*H*-pyran-3(6*H*)-one. Yield 398.4 mg, 83%. Conversion efficiency 88%. Yellow oil. TLC: Petroleum ether/EtOAc = 6/1, R_f = 0.6. 1H NMR (500 MHz, CDCl3) δ ppm: 7.28-7.27 (d, J = 8.2Hz, 2H), 6.91-6.89 (d, J = 8Hz, 2H), 6.80-6.78 (d, J = 10.4Hz, 1H), 6.15-6.13 (d, J = 10.35Hz, 1H), 4.66-4.56 (m, 3H), 4.18-4.14 (d, J = 16.95Hz, 1H), 3.87-3.81 (d, J = 30.3Hz, 3H), 3.63-3.61 (d, J = 9.95Hz, 1H), 3.55-3.53 (d, J = 10Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 194.8, 159.6, 145.7, 145.6, 132.0, 129.7, 129.1, 128.4, 128.0, 114.0, 113.9, 92.7, 73.8, 73.4, 67.9, 66.6, 55.5, 55.3. **HRMS (ESI$^+$):** calcd for $C_{14}H_{17}O_5$, $[M+H]^+$ 265.1071, found

265.1068.

B16: (2-hydroxy-5-oxo-5,6-dihydro-2H-pyran-2-yl)methyl acetate. Yield 348.2 mg, 76%. Conversion efficiency 87%. Yellow oil. TLC: Petroleum ether/EtOAc = 6/1, R_f = 0.35. **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm: 2.04-2.05(s, 3H), 4.56(s, 2H), 5.00(s, 2H), 6.22-6.23(d, 1H, *J* =2.9Hz), 6.32-6.33(d, 1H, *J* =2.95Hz). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 20.8, 57.4, 58.1, 108.5, 111.4, 149.4, 155.0, 170.7. **HRMS (ESI$^+$):** calcd for $C_8H_{11}O_5$, $[M+H]^+$ 187.0601, found 187.0658.

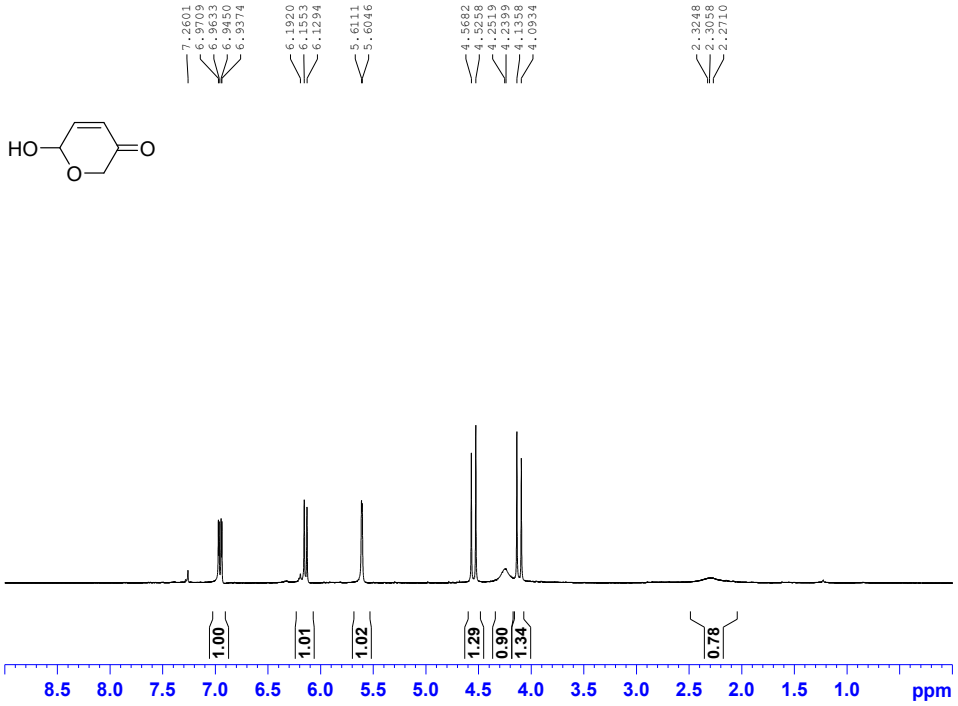
B17: (2-hydroxy-5-oxo-5,6-dihydro-2*H*-pyran-2-yl)methyl benzoate. Yield 390.3 mg, 82%. Conversion efficiency 86%. Yellow oil. TLC: Petroleum ether/EtOAc = 8/1, R_f = 0.5. 1H NMR (500 MHz, CDCl3) δ ppm: 8.07-8.03 (d, *J* = 18.35Hz, 2H), 7.63-7.60 (t, *J* = 14.85Hz, 1H), 7.49-7.42 (t, *J* = 31.7Hz, 2H), 7.03-7.01 (d, *J* = 10.4Hz, 1H), 6.22-6.20 (d, *J* = 10.4Hz, 1H), 4.70-4.63 (q, *J* = 33.65Hz, 2H), 4.38-4.34 (d, *J* = 21.3Hz, 1H), 4.24-4.21 (d, *J* = 16.95Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 194.3, 166.8, 145.0, 133.7, 129.9, 129.1, 128.6, 128.1, 92.5, 68.1, 66.6. **HRMS (ESI$^+$):** calcd for $C_{13}H_{13}O_5$, $[M+H]^+$ 249.0757, found 249.0755.

B18: (2-hydroxy-5-oxo-5,6-dihydro-2*H*-pyran-2-yl)methyl 4-methyl benzoate. Yield 376.0 mg, 80%. Conversion efficiency 85%. White solid. TLC: Petroleum ether/EtOAc = 7/1, R_f = 0.6. 1H NMR (500 MHz, CDCl3) δ ppm: 7.95-7.94 (d, *J* = 8.15Hz, 2H), 7.27-7.25 (d, *J* = 7.8Hz, 2H), 7.02-7.00 (d, *J* = 10.4Hz, 1H), 6.21-6.19 (d, *J* = 10.35Hz, 1H), 4.68-4.63 (t, *J* = 28Hz, 2H), 4.35-4.33 (d, *J* = 11.75Hz, 1H), 4.23-4.20 (d, *J* = 16.95Hz, 1H), 2.42 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 194.3, 166.9, 145.0, 144.6, 129.9, 129.3, 128.1, 126.3, 92.5, 67.9, 66.6, 21.8. **HRMS (ESI$^+$):** calcd for $C_{14}H_{15}O_5$, $[M+H]^+$ 263.0914, found 263.0917.

B19: (2-hydroxy-5-oxo-5,6-dihydro-2*H*-pyran-2-yl)methyl 4-methoxy benzoate. Yield 388.8 mg, 80%. Conversion efficiency 87%. White solid. TLC: Petroleum ether/EtOAc = 7/1, R_f = 0.6. 1H NMR (500 MHz, CDCl3) δ ppm: 8.001-7.99 (d, *J* = 8.5Hz, 2H), 7.01-6.99 (d, *J* = 10.35Hz, 1H), 6.94-6.92 (d, *J* = 8.4Hz, 2H), 6.20-6.18 (d, *J* = 10.4Hz, 12H), 4.65-4.62 (t, *J* = 17.8Hz, 2H), 4.34-4.31 (d, *J* = 11.8Hz, 1H), 4.22-4.19 (d, *J* = 16.95Hz, 1H), 3.98 (s, 1H), 3.86 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ ppm: 194.4, 166.6, 164.0, 145.2, 132.0, 128.0, 121.3, 113.9, 92.5, 67.9, 66.6, 55.5. HRMS (ESI$^+$): calcd for $C_{14}H_{15}O_6$, $[M+H]^+$ 279.0863, found 279.0869.

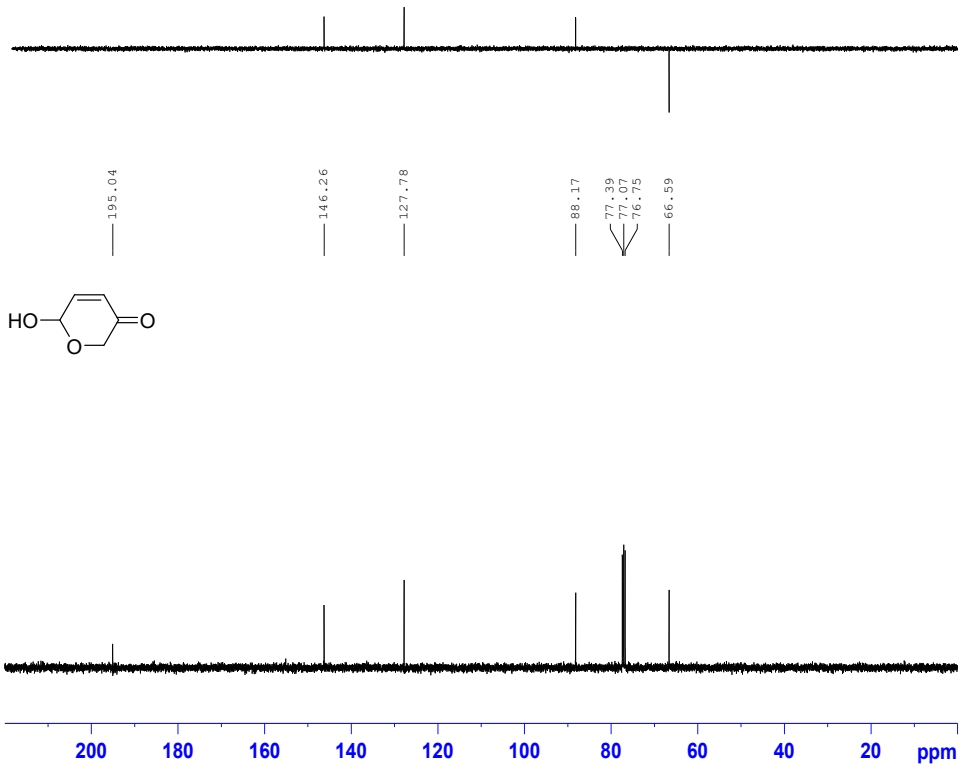
6.2 ^{1}H-NMR, ^{13}C-NMR, and 2D-NMR spectra

^{1}H-NMR (400 MHz, $CDCl_3$)



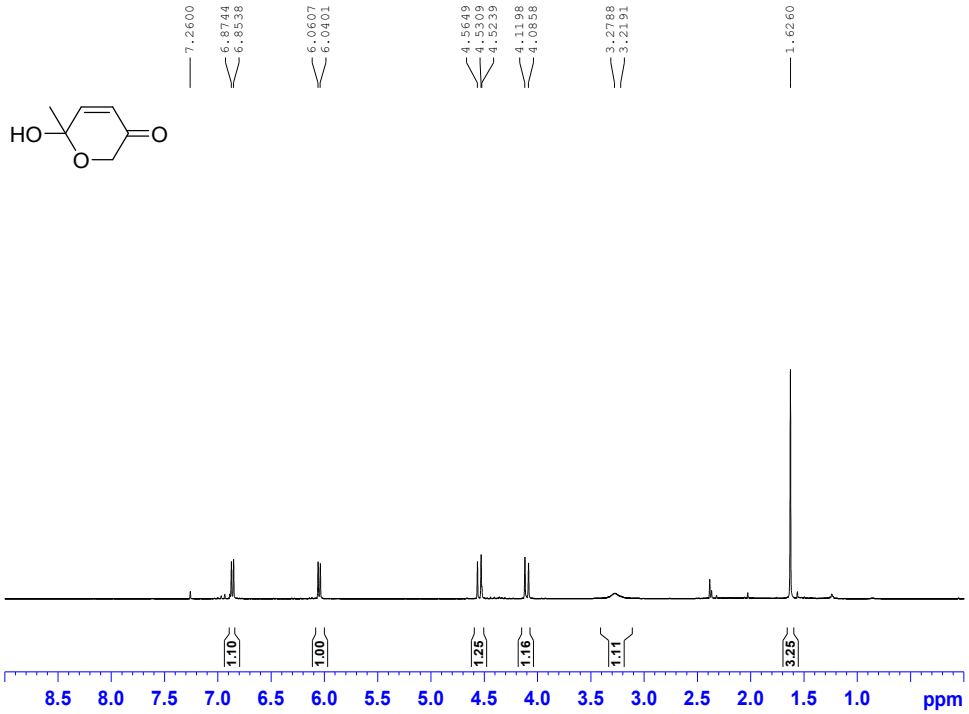

```
Current Data Parameters
NAME          bztyf01037
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180623
Time              22.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                24.66
DW              62.400 usec
DE                6.50 usec
TE               294.6 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1318812 MHz
NUC1                  1H
P1                12.00 usec
PLW1        11.69999981 W

F2 - Processing parameters
SI                65536
SF           400.1300096 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
bztyf01037
```

^{13}C-NMR (100 MHz, $CDCl_3$)




```
Current Data Parameters
NAME          bztyf01037
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180623
Time              22.57
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                    5
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                214.83
DW              20.800 usec
DE                6.50 usec
TE               295.0 K
D1           3.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6240376 MHz
NUC1                 13C
P1                12.00 usec
PLW1        51.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        11.69999981 W
PLW12        0.26324999 W
PLW13        0.16847999 W

F2 - Processing parameters
SI                32768
SF           100.6127690 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
bztyf01037
```

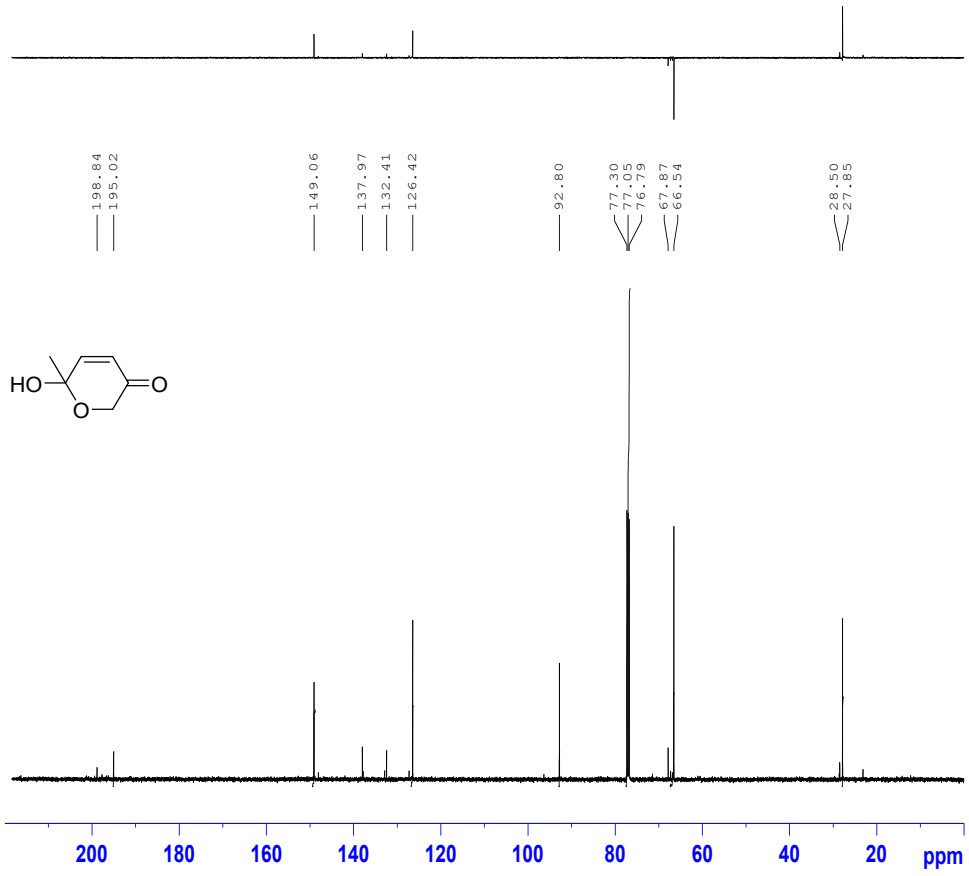
^{1}H-NMR (500 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20220311 nmr ynu
EXPNO               10
PROCNO               1

F2 - Acquisition Parameters
Date_          20220311
Time              15.43 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               69.86
DW               50.000 usec
DE               13.89 usec
TE               295.5 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300119 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
```

TYF04086-1

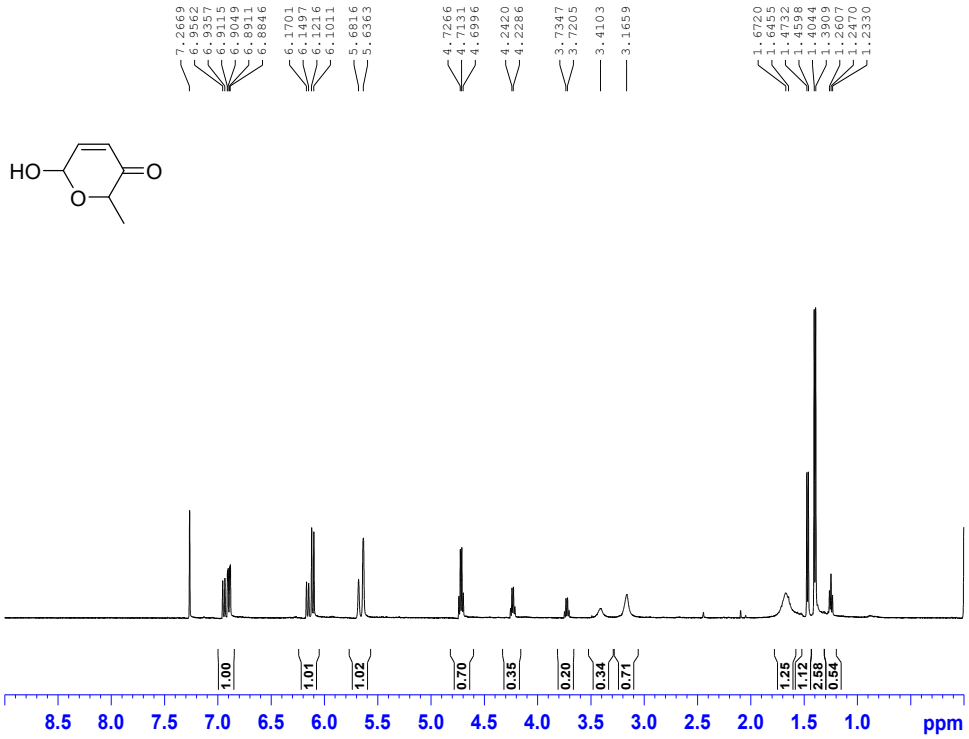
^{13}C-NMR (125 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20220311 nmr c
EXPNO               12
PROCNO               1

F2 - Acquisition Parameters
Date_          20220314
Time              15.50 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 180
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```

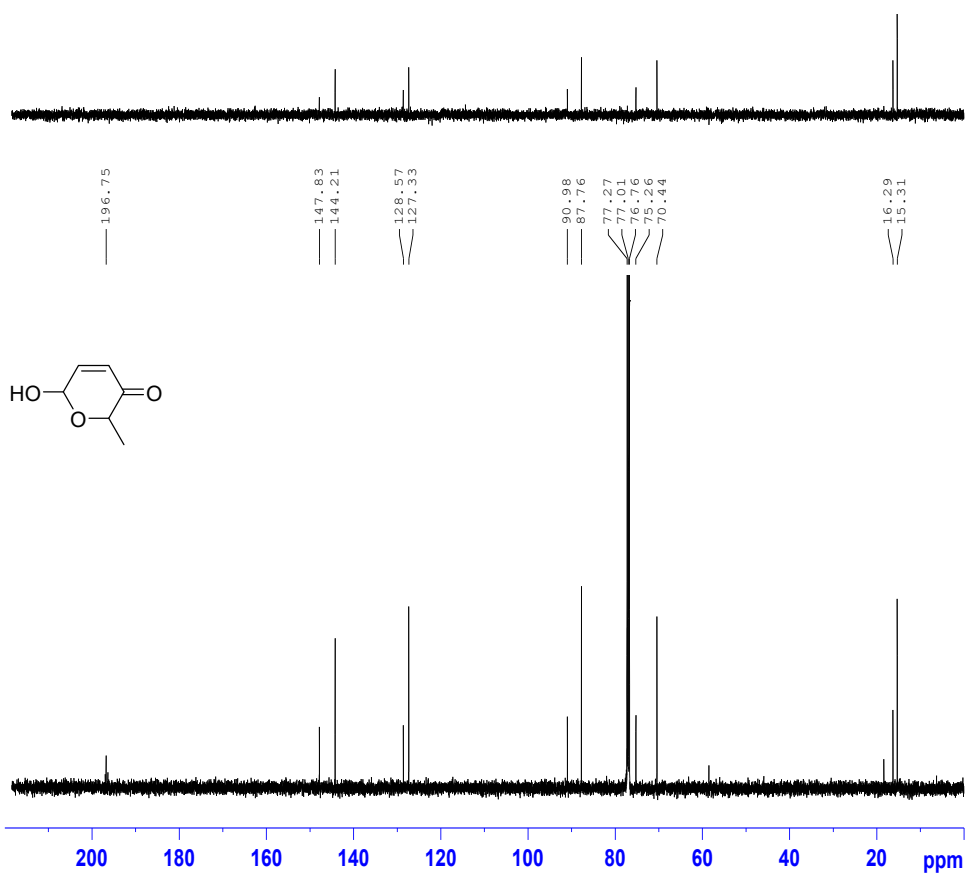
TYF04086-1

^{1}H-NMR (500 MHz, $CDCl_3$)



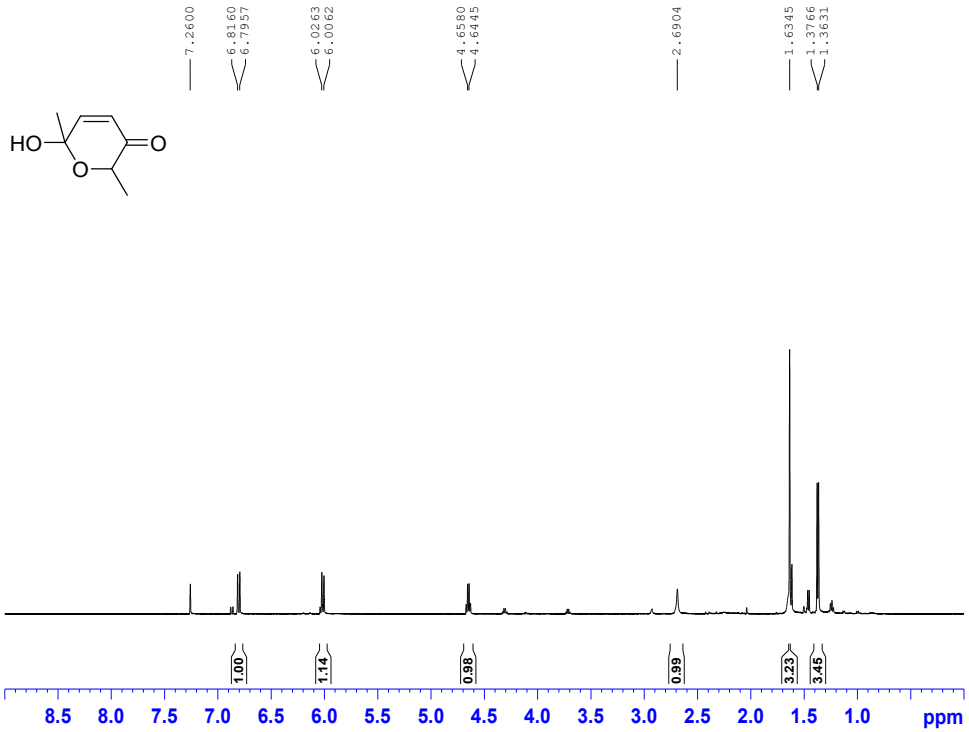

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO               10
PROCNO               1

F2 - Acquisition Parameters
Date_          20220322
Time              16.26 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                152.21
DW                50.000 usec
DE                13.89 usec
TE                295.8 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300086 MHz
WDW                 EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
TYF04095-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



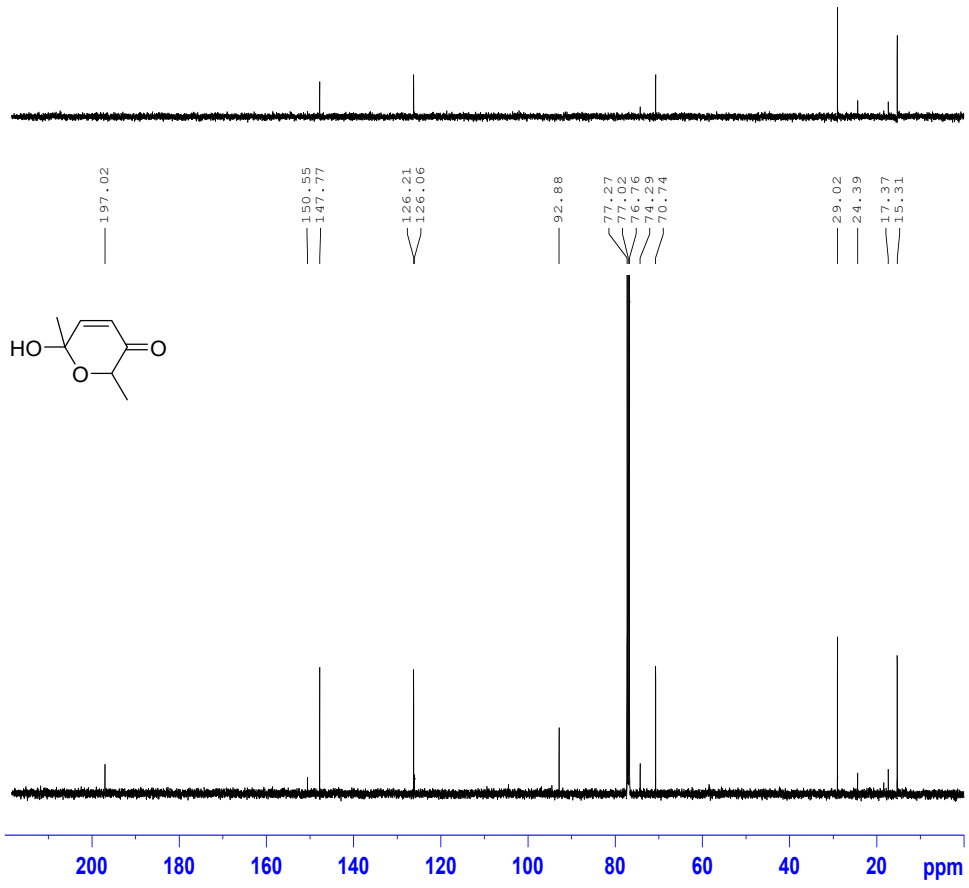

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO               12
PROCNO               1

F2 - Acquisition Parameters
Date_          20220322
Time              16.58 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 400
DS                   4
SWH           29761.904 Hz
FIDRES            0.908261 Hz
AQ             1.1010048 sec
RG                190.79
DW                16.800 usec
DE                 6.50 usec
TE                296.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                 13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
TYF04095-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



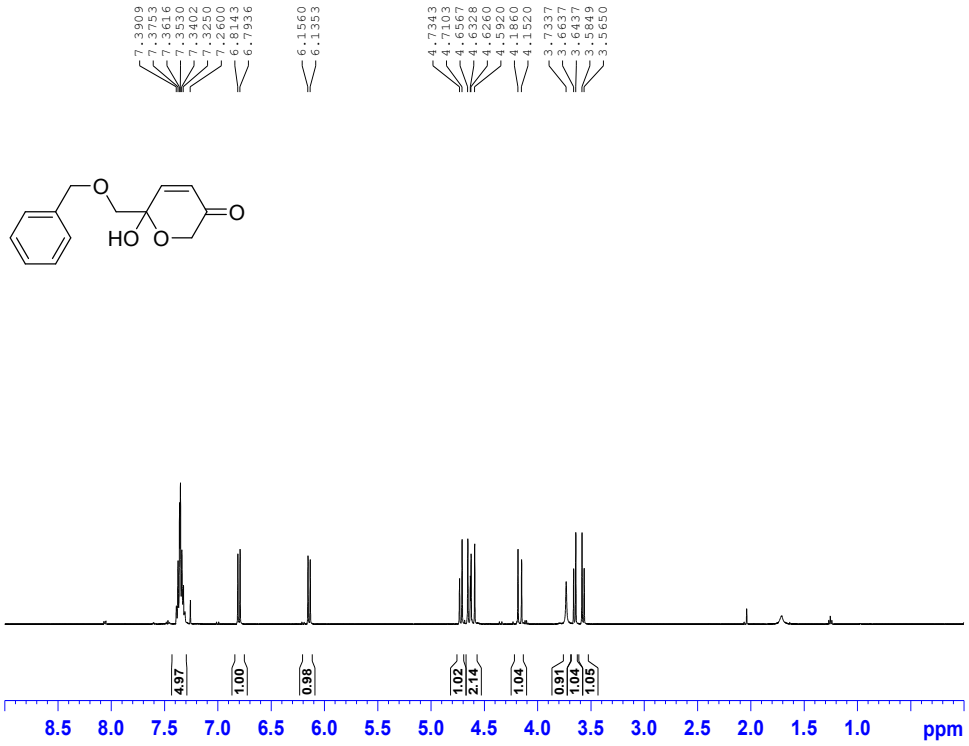

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO               50
PROCNO               1

F2 - Acquisition Parameters
Date_          20220322
Time              17.46 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               116.68
DW               50.000 usec
DE                13.89 usec
TE                296.4 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300118 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
TYF04099-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



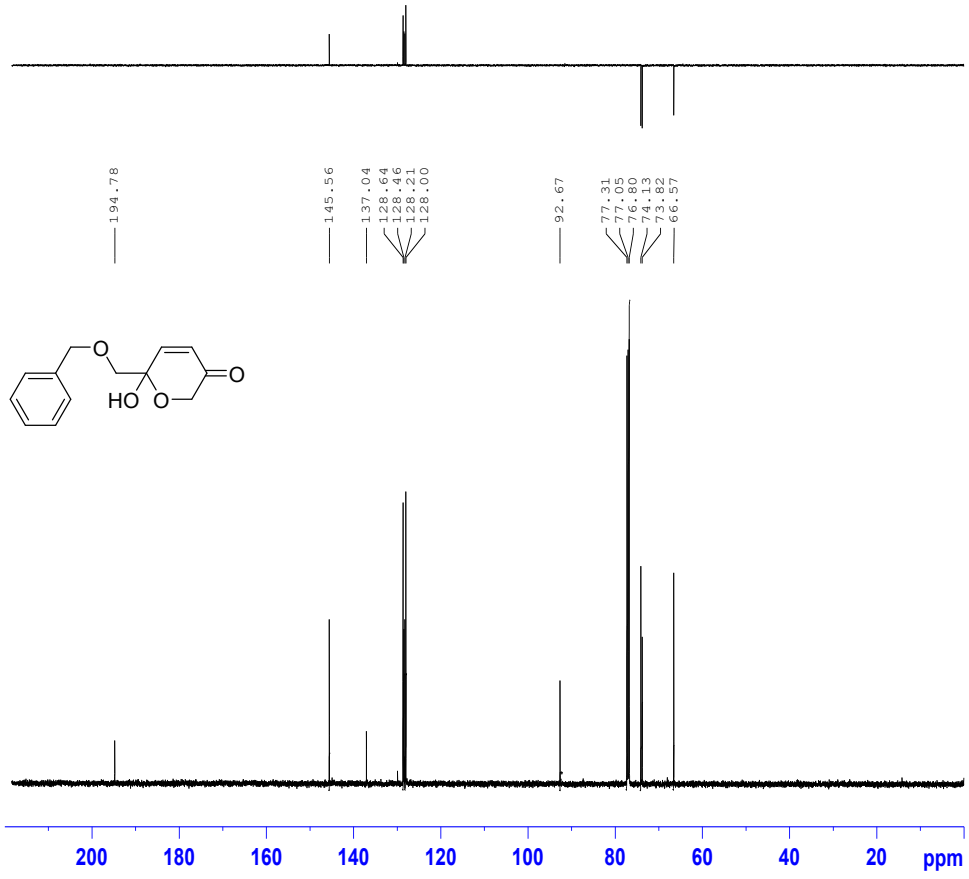

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO               52
PROCNO               1

F2 - Acquisition Parameters
Date_          20220322
Time              17.59 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 240
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE                296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
TYF04099-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



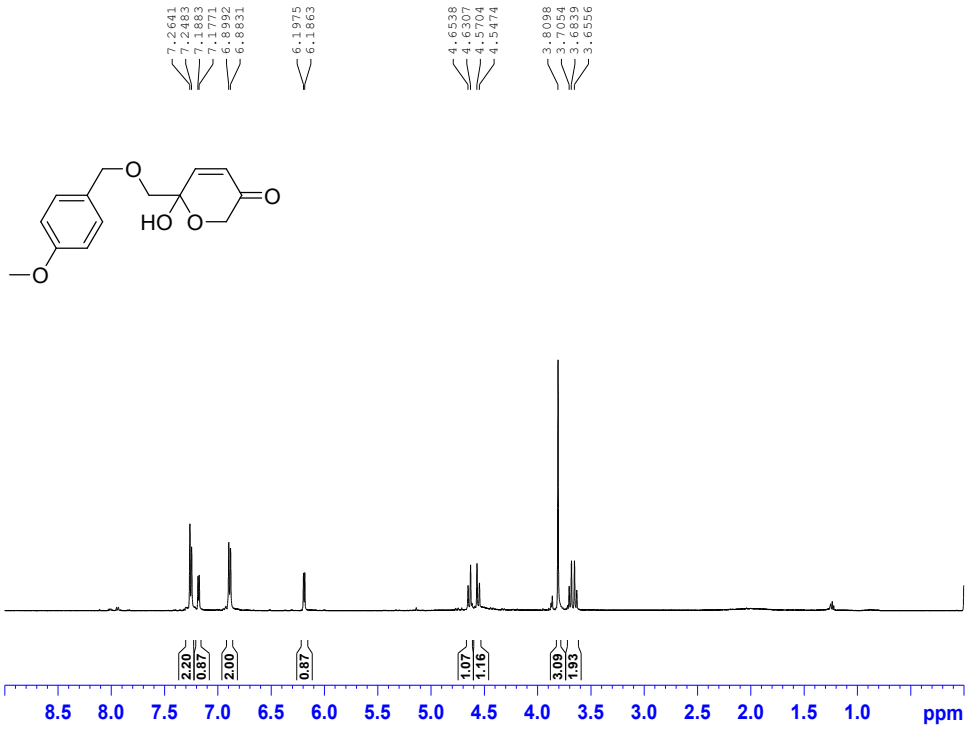

```
Current Data Parameters
NAME       20220407 nmr
EXPNO              100
PROCNO               1

F2 - Acquisition Parameters
Date_           20220407
Time              16.33 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                76.76
DW               50.000 usec
DE               13.89 usec
TE               293.1 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300124 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
TYF04106-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



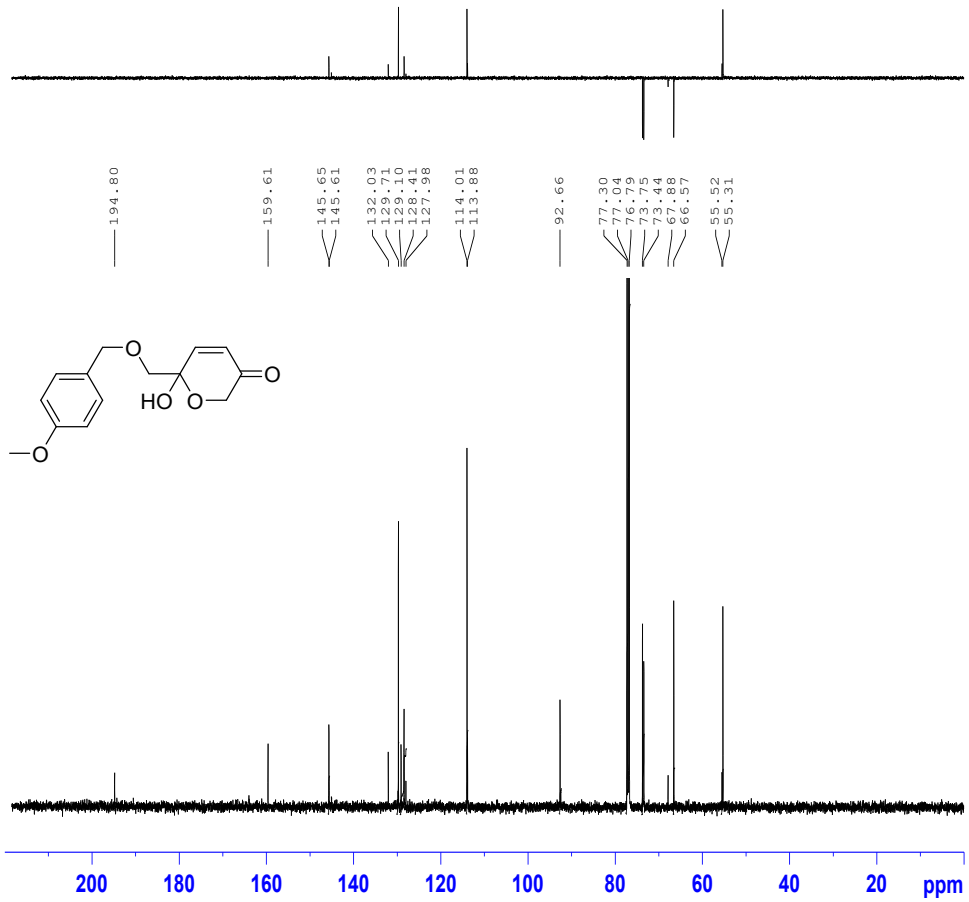

```
Current Data Parameters
NAME     20220407 nmr c
EXPNO              102
PROCNO               1

F2 - Acquisition Parameters
Date_           20220408
Time              3.18 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 160
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               294.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
TYF04106-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



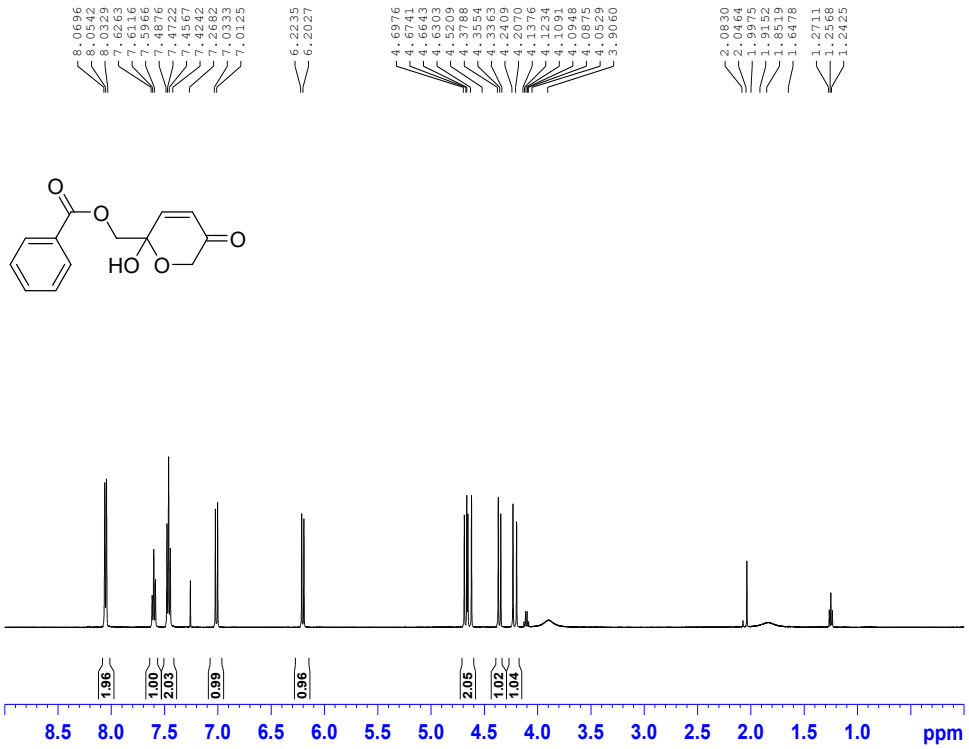

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO               40
PROCNO               1

F2 - Acquisition Parameters
Date_          20220322
Time              17.29 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               116.68
DW               50.000 usec
DE               13.89 usec
TE               296.4 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300103 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
TYF04098-2
```

^{13}C-NMR (125 MHz, $CDCl_3$)



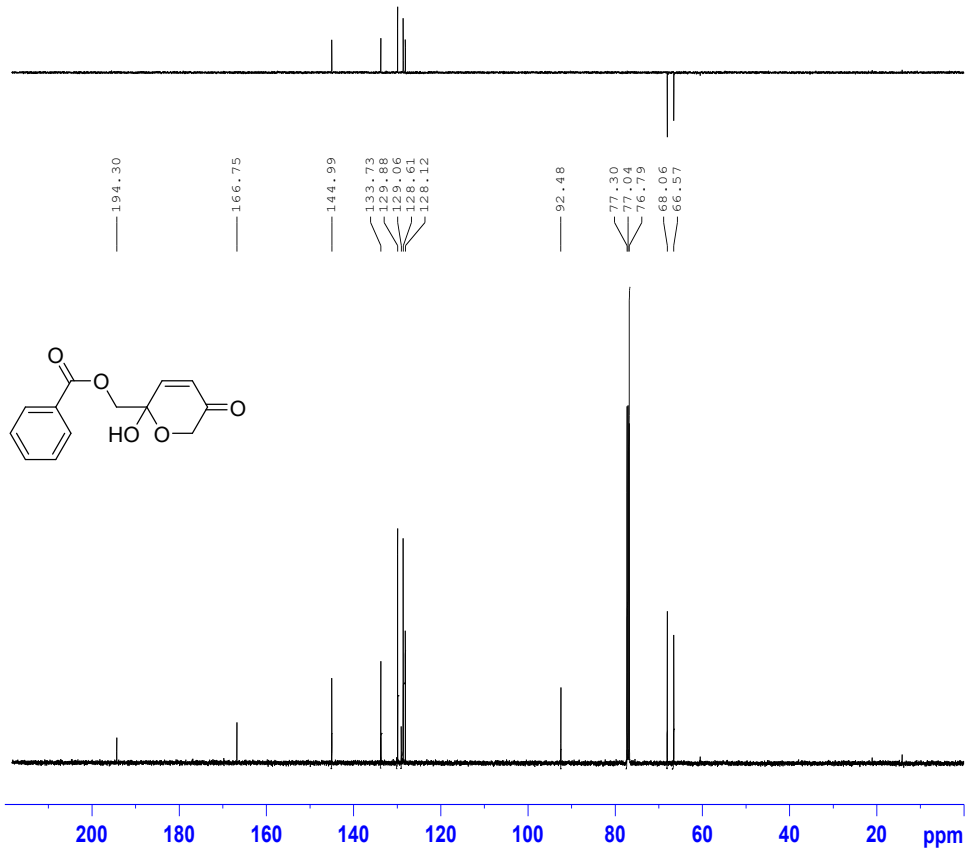

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO               31
PROCNO               1

F2 - Acquisition Parameters
Date_          20220322
Time              17.24 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 106
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               296.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB               1.70 Hz
GB       0
PC               1.40
TYF04098-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



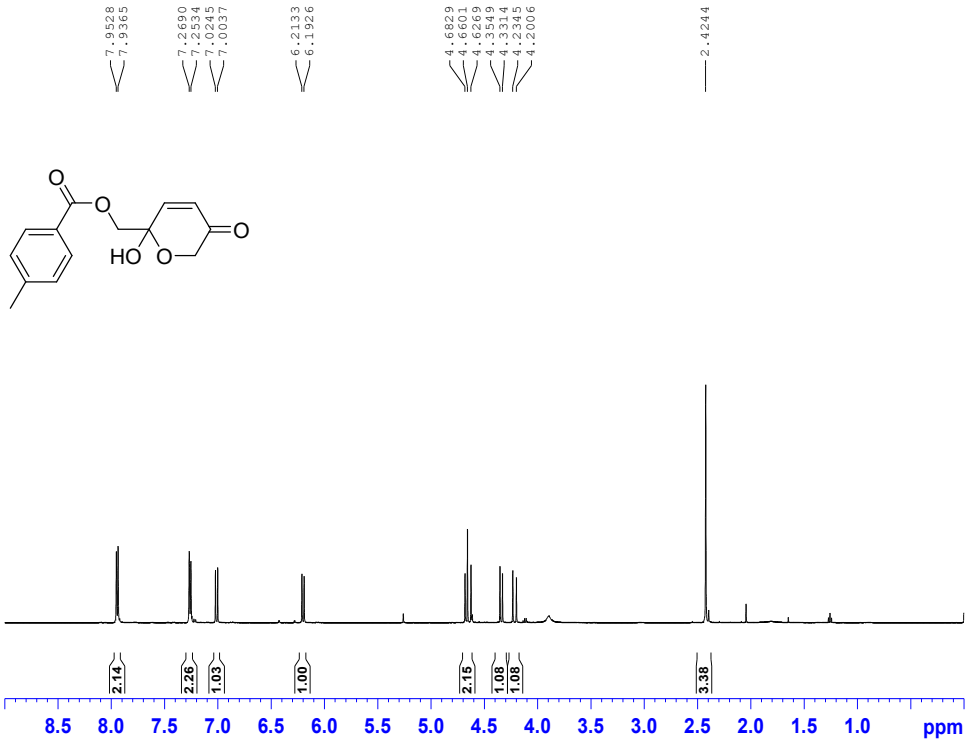

```
Current Data Parameters
NAME       20220407 nmr
EXPNO                90
PROCNO                1

F2 - Acquisition Parameters
Date_          20220407
Time              16.31 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                95.16
DW               50.000 usec
DE               13.89 usec
TE               293.1 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300124 MHz
WDW                 EM
SSB       0
LB             0.30 Hz
GB        0
PC             1.00
TYF04105-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



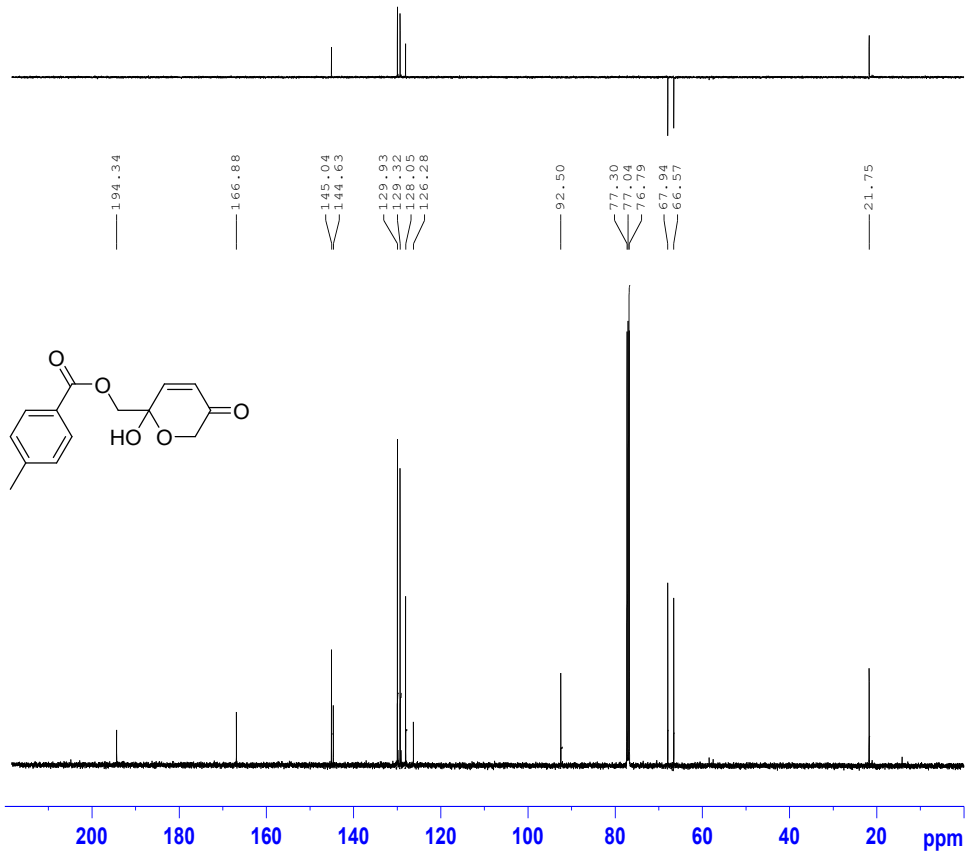

```
Current Data Parameters
NAME     20220407 nmr c
EXPNO                92
PROCNO                1

F2 - Acquisition Parameters
Date_          20220408
Time              3.04 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 180
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB       0
LB             1.00 Hz
GB        0
PC             1.40
TYF04105-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



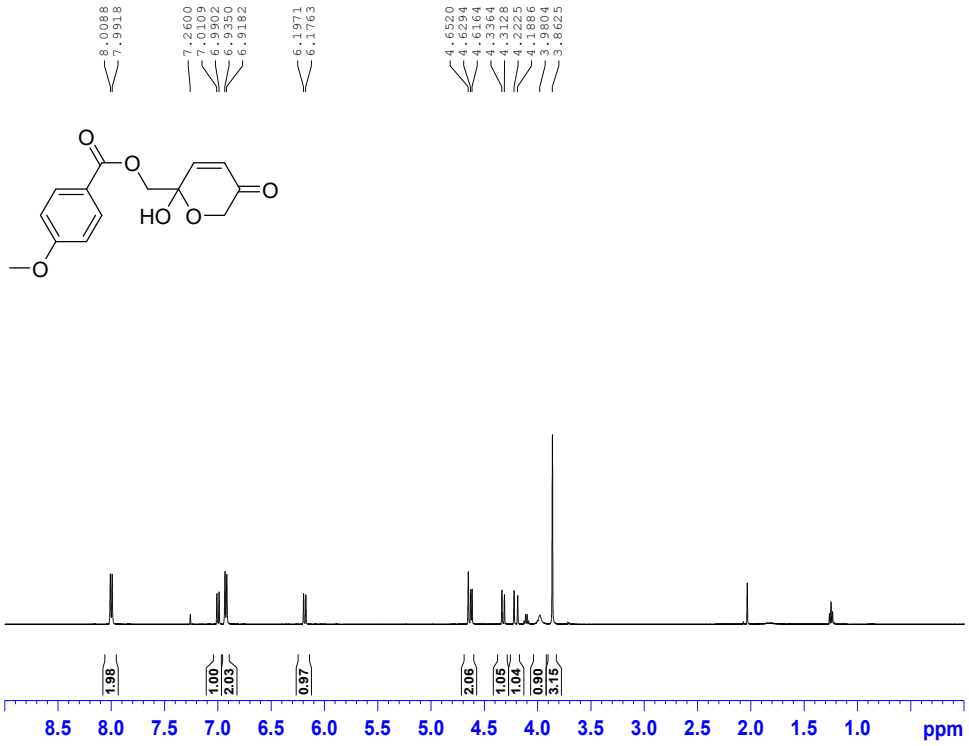

```
Current Data Parameters
NAME       20220407 nmr
EXPNO               110
PROCNO                1

F2 - Acquisition Parameters
Date_          20220407
Time              16.35 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                    2
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                86.69
DW               50.000 usec
DE               13.89 usec
TE                293.1 K
D1           1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI                65536
SF          500.1300088 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
TYF04107-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



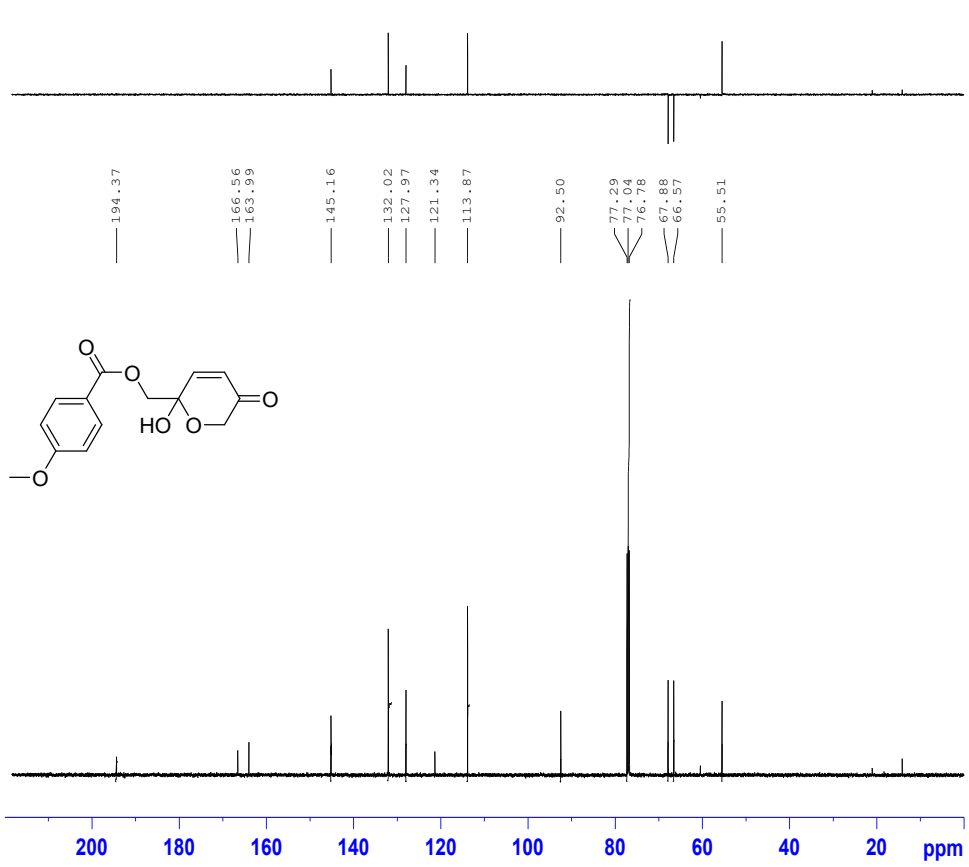

```
Current Data Parameters
NAME      20220407 nmr c
EXPNO               112
PROCNO                1

F2 - Acquisition Parameters
Date_          20220408
Time              3.32 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                  180
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE                294.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI                32768
SF          125.7577885 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
TYF04107-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



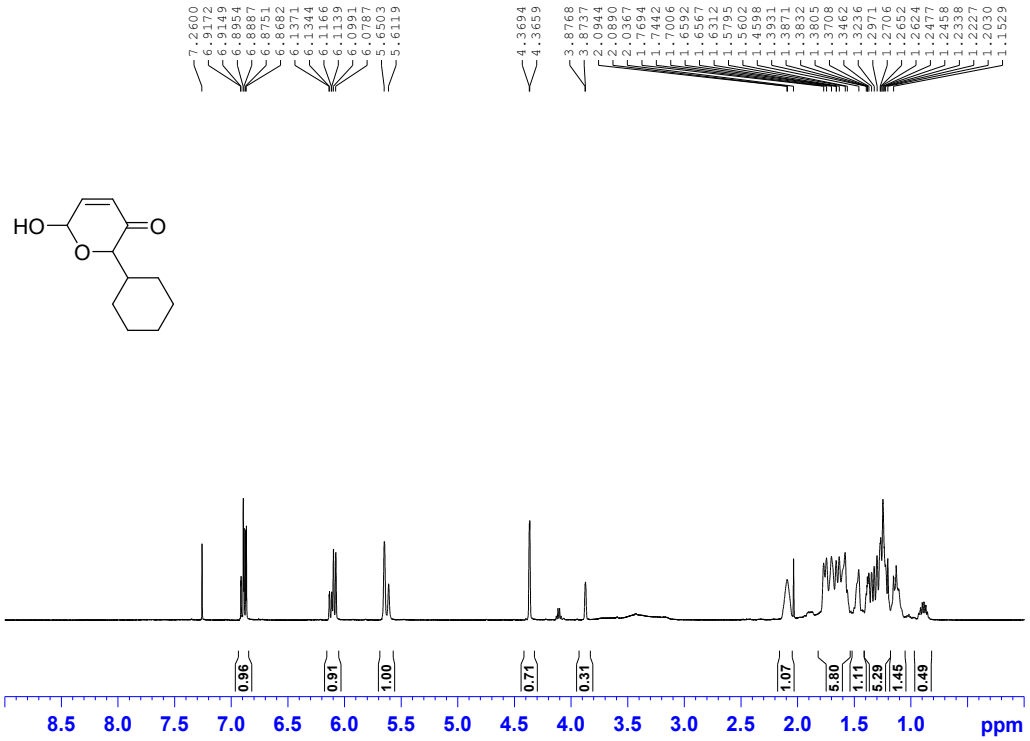

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_          20220322
Time              17.06 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    2
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                76.76
DW               50.000 usec
DE                13.89 usec
TE                296.5 K
D1           1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI                65536
SF          500.1300118 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
TYF04096-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



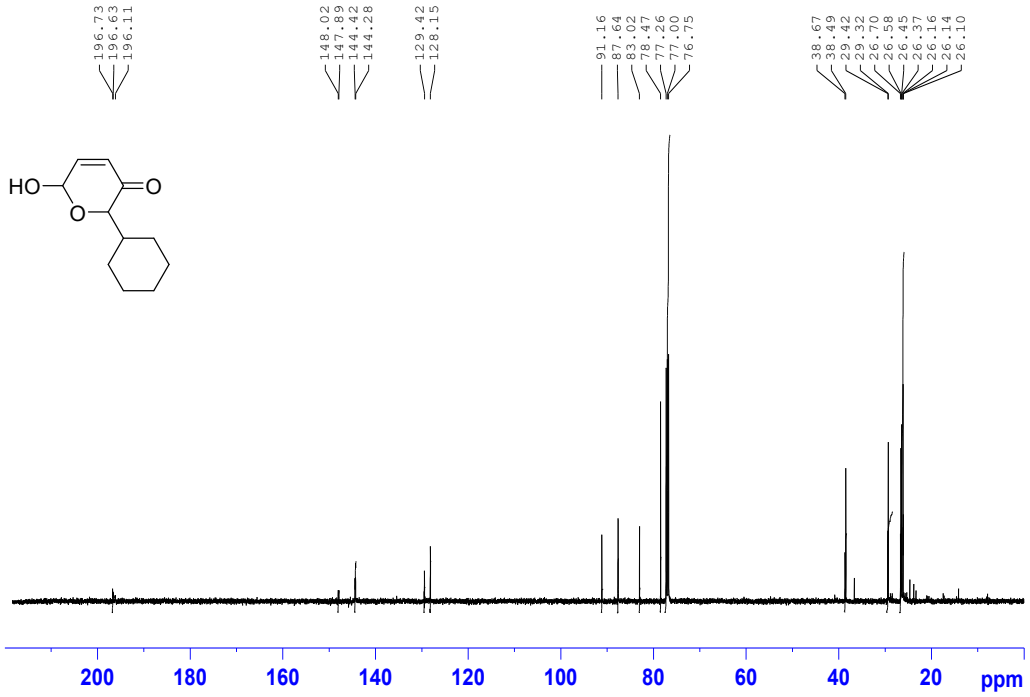

```
Current Data Parameters
NAME      20220322 nmr h
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20220322
Time              17.13 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  123
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE                296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI                32768
SF          125.7577885 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
TYF04096-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



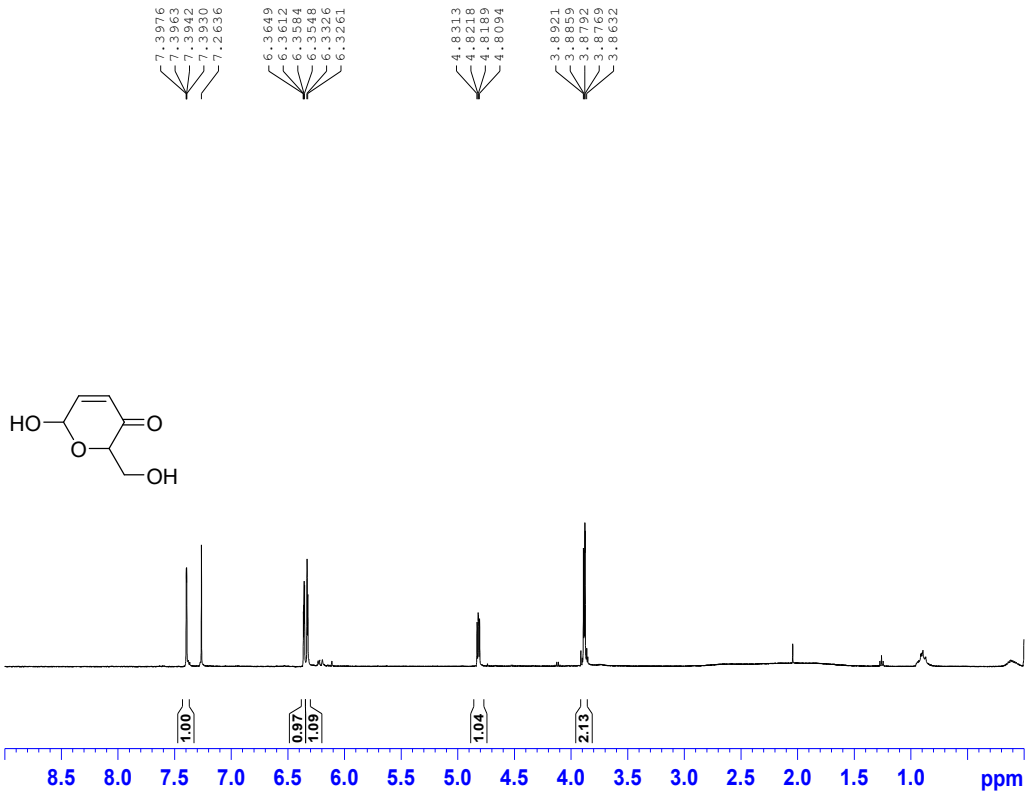

```
Current Data Parameters
NAME      20220922 nmr h
EXPNO               10
PROCNO               1

F2 - Acquisition Parameters
Date_          20220922
Time              15.21 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                69.86
DW                50.000 usec
DE                13.89 usec
TE                298.7 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300121 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
TYF04178-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



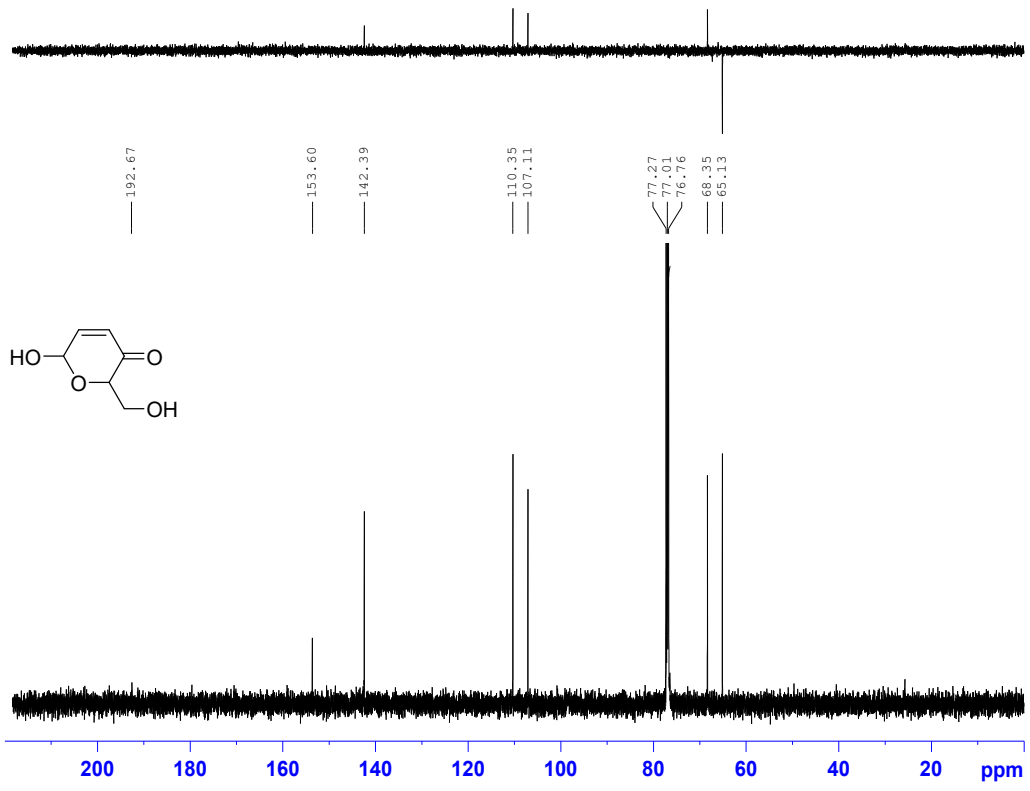

```
Current Data Parameters
NAME      20220922 nmr c
EXPNO               12
PROCNO               1

F2 - Acquisition Parameters
Date_          20220924
Time              0.43 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 400
DS                   4
SWH           29761.904 Hz
FIDRES            0.908261 Hz
AQ             1.1010048 sec
RG                190.79
DW                16.800 usec
DE                 6.50 usec
TE                303.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI                32768
SF           125.7577885 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
TYF04178-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



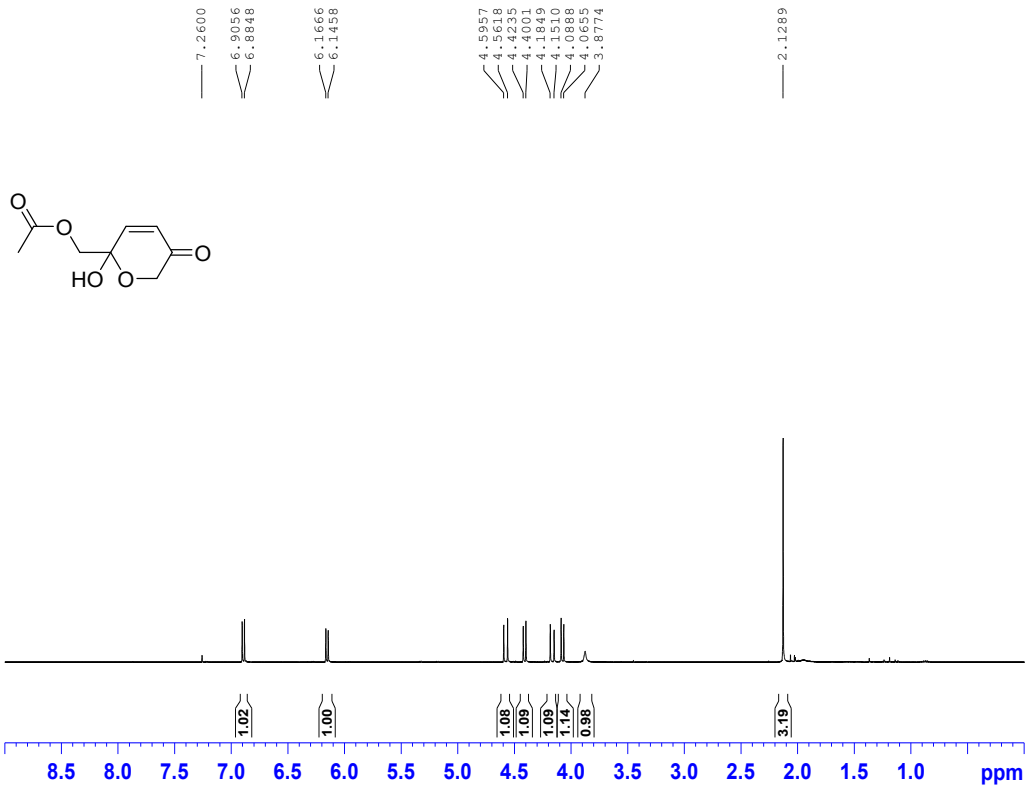

```
Current Data Parameters
NAME      20220908 nmr h
EXPNO                70
PROCNO                1

F2 - Acquisition Parameters
Date_          20220908
Time              12.42 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG               152.21
DW               50.000 usec
DE               13.89 usec
TE               298.6 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI               65536
SF           500.1300102 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
tyf04172-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



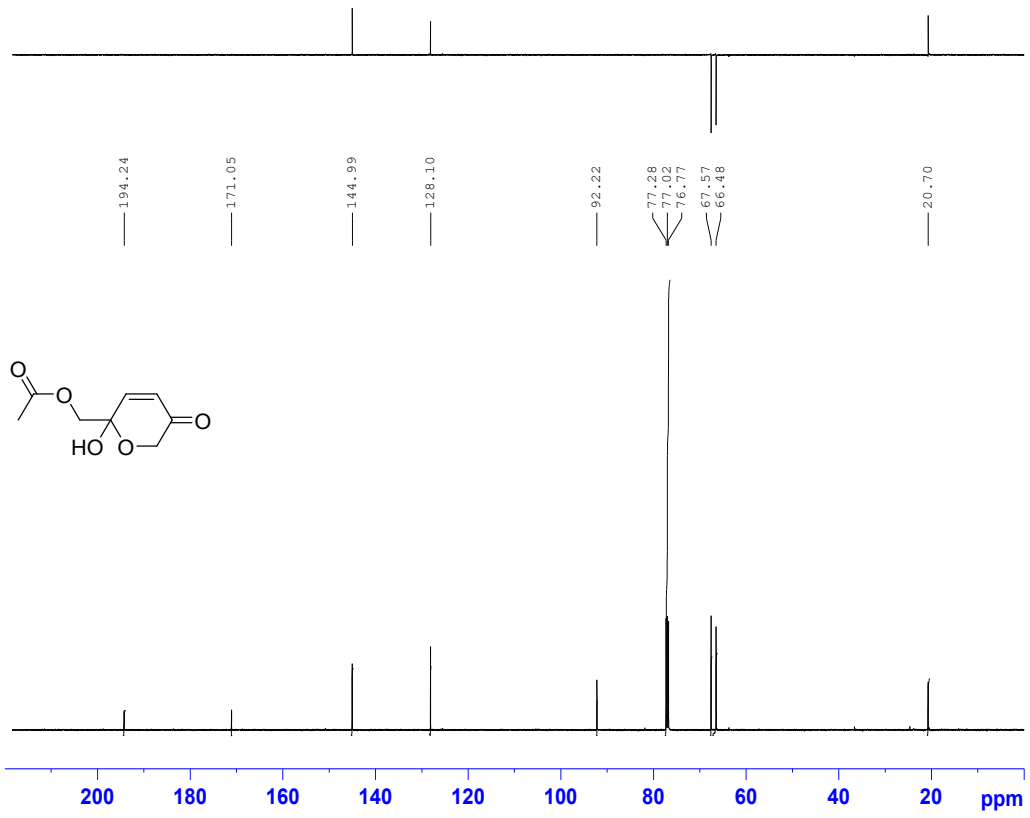

```
Current Data Parameters
NAME      20220908 nmr c
EXPNO                72
PROCNO                1

F2 - Acquisition Parameters
Date_          20220908
Time              18.31 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               299.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1         125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI               32768
SF           125.7577885 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
tyf04172-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



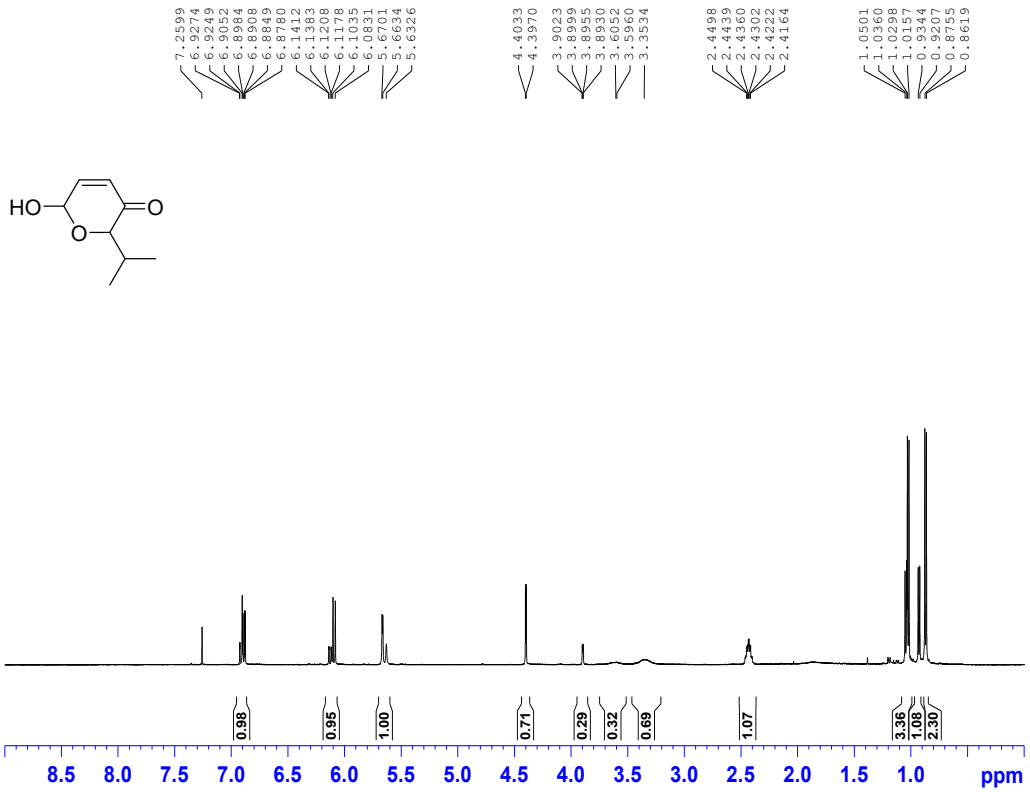

```
Current Data Parameters
NAME        20221008 nmr
EXPNO               11
PROCNO               1

F2 - Acquisition Parameters
Date_           20221008
Time              11.50 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   4
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                76.76
DW               50.000 usec
DE               13.89 usec
TE               304.3 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                 1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI               65536
SF          500.1300118 MHz
WDW                 EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
TYF04182-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



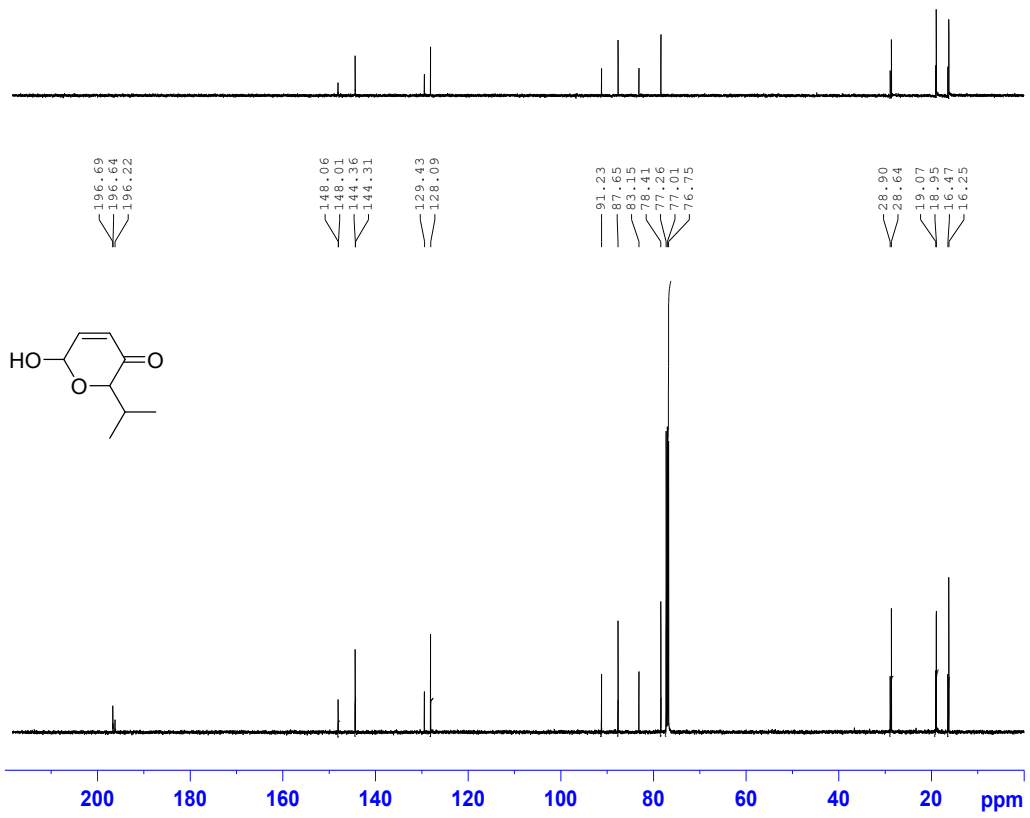

```
Current Data Parameters
NAME        20221008 nmr
EXPNO               12
PROCNO               1

F2 - Acquisition Parameters
Date_           20221008
Time              12.04 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               305.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI               32768
SF          125.7577885 MHz
WDW                 EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
TYF04182-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



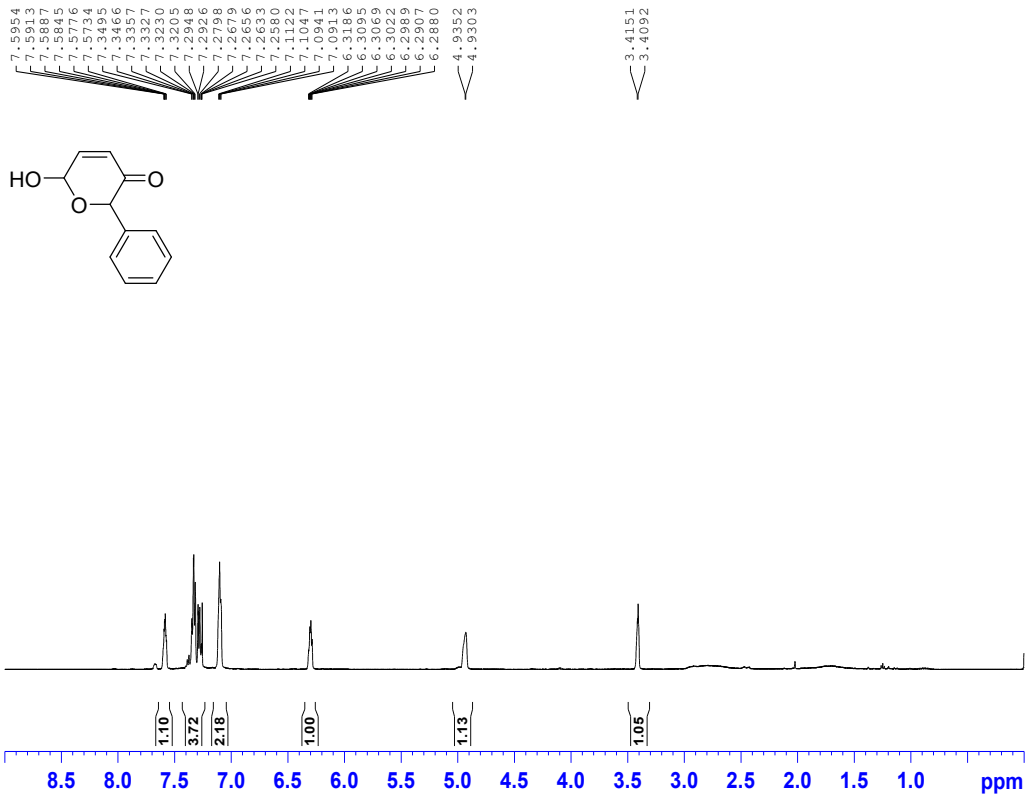

```
Current Data Parameters
NAME      20220922 nmr h
EXPNO                40
PROCNO                1

F2 - Acquisition Parameters
Date_            20220922
Time               15.35 h
INSTRUM             spect
PROBHD    Z113652_0230 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      2
DS                      2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ              3.2767999 sec
RG                  76.76
DW                50.000 usec
DE                13.89 usec
TE                299.0 K
D1            1.00000000 sec
TD0                     1
SFO1         500.1330883 MHz
NUC1                   1H
P0                  3.33 usec
P1                 10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI                  65536
SF           500.1300124 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
TYF04177-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)



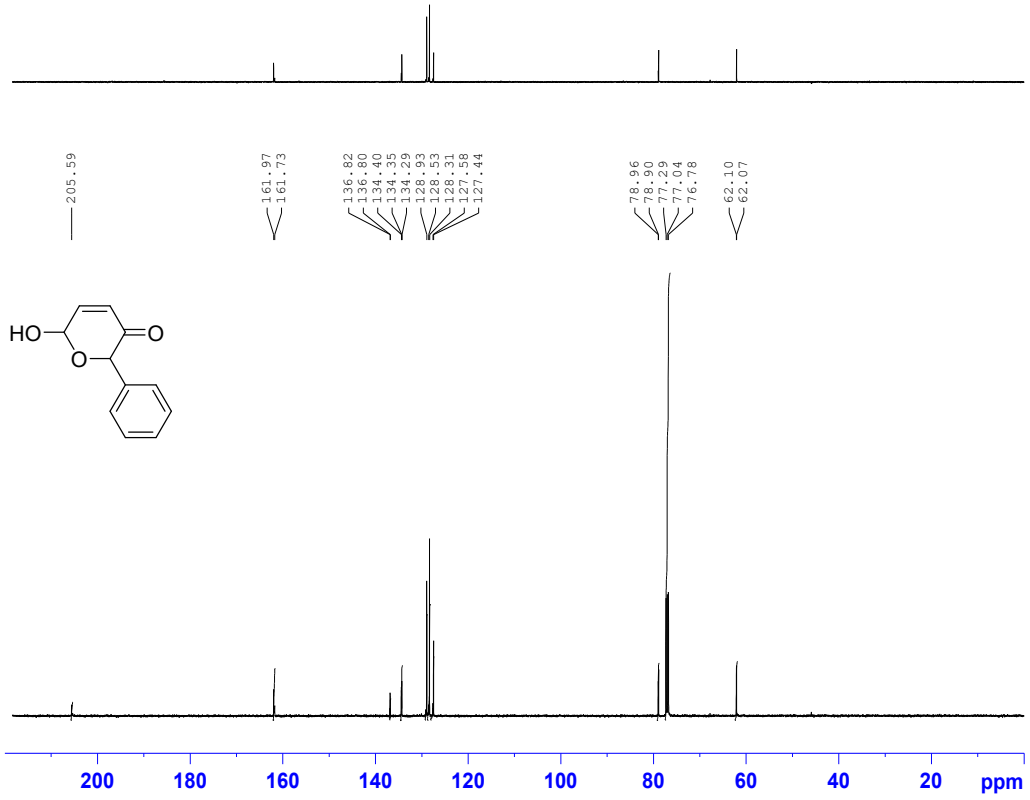

```
Current Data Parameters
NAME      20220922 nmr c
EXPNO                42
PROCNO                1

F2 - Acquisition Parameters
Date_            20220924
Time                2.02 h
INSTRUM             spect
PROBHD    Z113652_0230 (
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    400
DS                      4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                 190.79
DW                16.800 usec
DE                 6.50 usec
TE                302.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         125.7703643 MHz
NUC1                  13C
P0                  3.33 usec
P1                 10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                   1H
CPDPRG[2         waltz65
PCPD2              80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI                  32768
SF           125.7577885 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
TYF04177-1
```

^{1}H-NMR (500 MHz, $CDCl_3$)



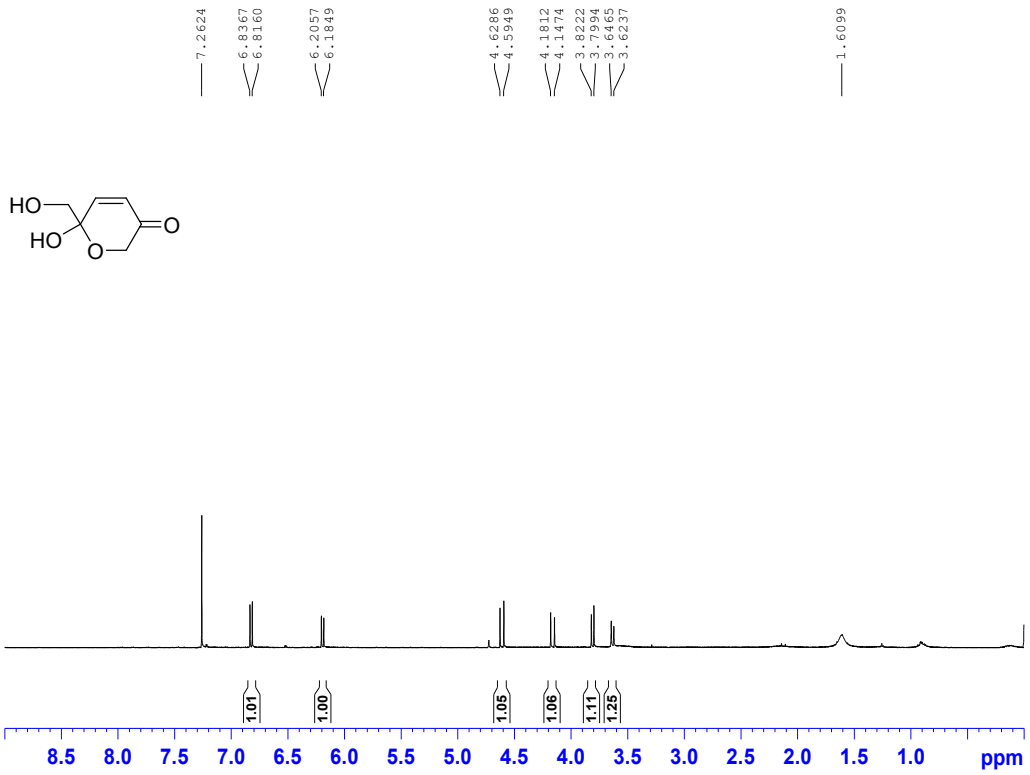

```
Current Data Parameters
NAME      20220922 nmr h
EXPNO               50
PROCNO               1

F2 - Acquisition Parameters
Date_           20220922
Time              15.40 h
INSTRUM           spect
PROBHD    Z113652_0230 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     2
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                95.16
DW               50.000 usec
DE               13.89 usec
TE               299.0 K
D1            1.00000000 sec
TD0                    1
SFO1         500.1330883 MHz
NUC1                  1H
P0                 3.33 usec
P1                10.00 usec
PLW1         25.23200035 W

F2 - Processing parameters
SI                 65536
SF           500.1300133 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
TYF04176-2
```

^{13}C-NMR (125 MHz, $CDCl_3$)



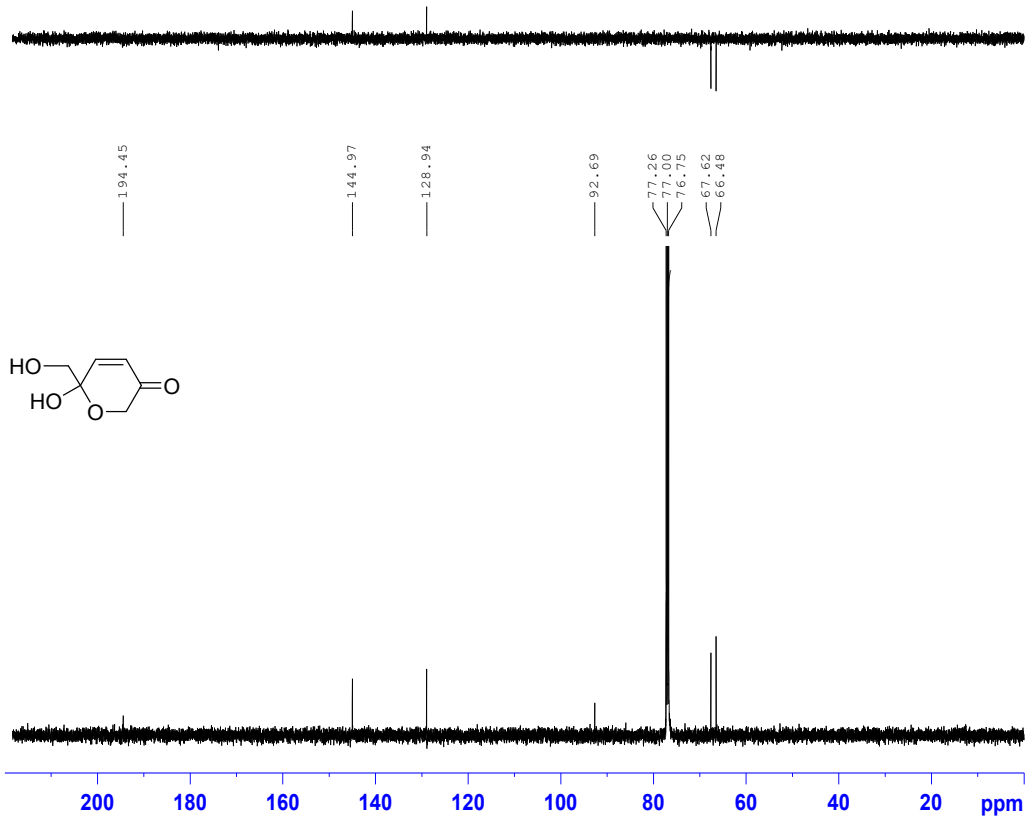

```
Current Data Parameters
NAME      20220922 nmr c
EXPNO               52
PROCNO               1

F2 - Acquisition Parameters
Date_           20220924
Time              2.33 h
INSTRUM           spect
PROBHD    Z113652_0230 (
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   400
DS                     4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                190.79
DW               16.800 usec
DE                6.50 usec
TE               303.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P0                 3.33 usec
P1                10.00 usec
PLW1        102.87999725 W
SFO2         500.1320005 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         25.23200035 W
PLW12         0.39425001 W
PLW13         0.19831000 W

F2 - Processing parameters
SI                 32768
SF           125.7577885 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
TYF04176-2
```

^{1}H-NMR (500 MHz, $CDCl_3$)



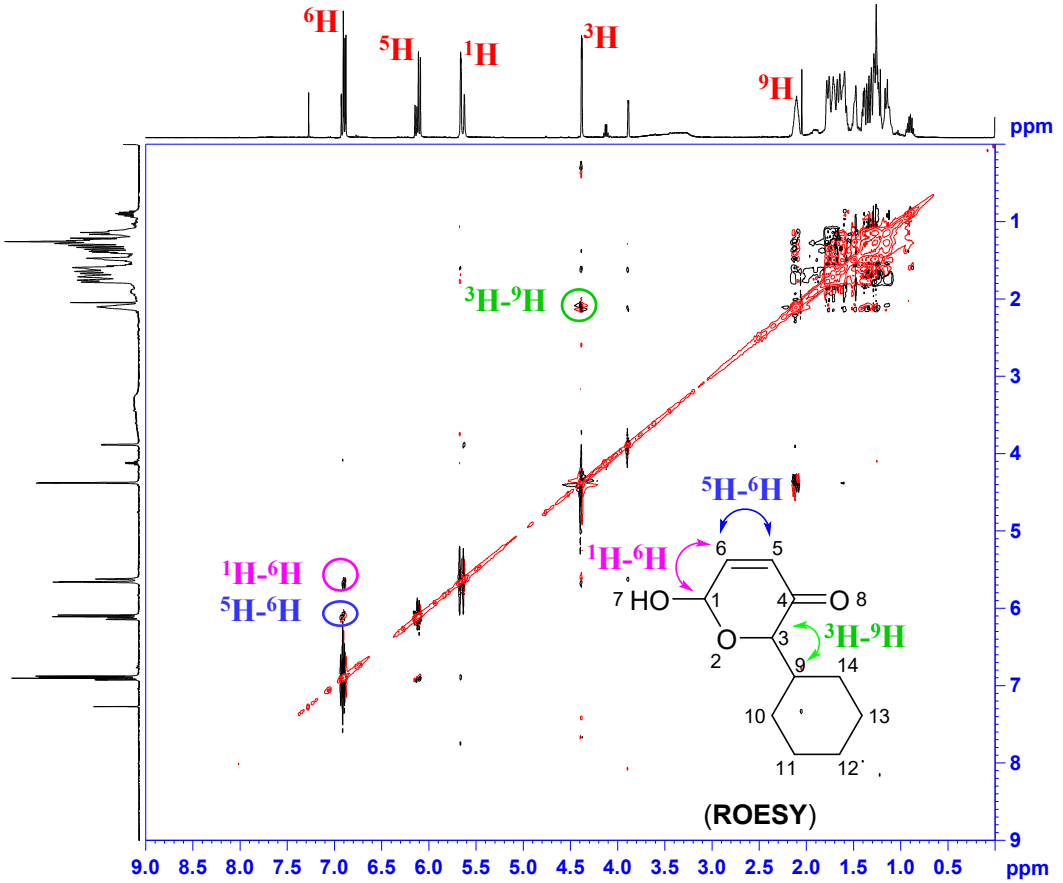

```
Current Data Parameters
NAME      20220908 nmr h
EXPNO               10
PROCNO               1

F2 - Acquisition Parameters
Date_          20220908
Time              12.31 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   2
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               190.79
DW               50.000 usec
DE               13.89 usec
TE               299.0 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P0                3.33 usec
P1               10.00 usec
PLW1        25.23200035 W

F2 - Processing parameters
SI                65536
SF           500.1300109 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
tyf04167-1
```

^{13}C-NMR (125 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      20220908 nmr c
EXPNO               15
PROCNO               1

F2 - Acquisition Parameters
Date_          20220908
Time              17.54 h
INSTRUM           spect
PROBHD   Z113652_0230 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 580
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               190.79
DW               16.800 usec
DE                6.50 usec
TE               299.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1       102.87999725 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            80.00 usec
PLW2        25.23200035 W
PLW12        0.39425001 W
PLW13        0.19831000 W

F2 - Processing parameters
SI                32768
SF           125.7577885 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
tyf04167-1
```

2D-NMR (ROESY)




```
Current Data Parameters
NAME        20220922 nmr c
EXPNO                   13
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220924
Time_               1.27
INSTRUM             spect
PROBHD    Z113652_0230 (
PULPROG     roesyphpp.2
TD                  2048
SOLVENT             CDCl3
NS                     4
DS                    32
SWH             5000.000 Hz
FIDRES          2.441406 Hz
AQ              0.2048000 sec
RG                  36.98
DW                100.000 usec
DE                  6.50 usec
TE                 303.4 K
d0             -0.00001037 sec
D1              2.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec
in0       0 sec
14                    463
P15            200000.00 usec
ST1CNT                 0
d0orig         -0.00001037 sec
ph1loop                0
tl1oop                 0
SFO1          500.1323506 MHz
NUC1                  1H
P1                 10.00 usec
P17              2500.00 usec
P25               216.00 usec
PLW1          25.23200035 W
PLW10          2.80360007 W
PLW27          0.21633001 W

F1 - Acquisition parameters
TD                    256
SFO1          500.1324 MHz
FIDRES         19.531250 Hz
SW                 9.997 ppm
FnMODE        States-TPPI

F2 - Processing parameters
SI                   1024
SF            500.1300000 MHz
WDW                  QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.00

F1 - Processing parameters
SI                   1024
MC2           States-TPPI
SF            500.1300000 MHz
WDW                  QSINE
SSB                     2
LB        0 Hz
GB        0
```

7. *In-situ* IR original data

reaction time	time (min)	[reactant]	-ln [product]	[product]	reaction temperature
0:26:40	26.67	0.09552	9.04992	0.000117	35.00
0:27:25	27.42	0.09855	8.97017	0.000127	35.08
0:28:10	28.17	0.09773	9.07527	0.000114	34.87
0:28:55	28.92	0.09617	9.18729	0.000102	40.35
0:29:40	29.67	0.09627	9.62692	0.000066	39.68
0:30:25	30.42	0.09601	9.53010	0.000073	39.73
0:31:10	31.17	0.09629	9.46721	0.000077	39.38
0:31:55	31.92	0.09609	9.59138	0.000068	39.10
0:32:40	32.67	0.09660	9.17213	0.000104	39.16
0:33:25	33.42	0.09700	9.11869	0.000110	39.13
0:34:10	34.17	0.09615	9.05209	0.000117	39.10
0:34:55	34.92	0.09677	9.14124	0.000107	39.12
0:35:40	35.67	0.09685	9.31530	0.000090	39.17
0:36:25	36.42	0.09601	9.04377	0.000118	39.06
0:37:10	37.17	0.09681	8.86753	0.000141	39.13
0:37:55	37.92	0.09553	9.10192	0.000111	39.32
0:38:40	38.67	0.09643	8.79391	0.000152	39.05
0:39:25	39.42	0.09593	8.74580	0.000159	39.37
0:40:10	40.17	0.09639	8.89867	0.000137	39.52
0:40:55	40.92	0.09621	8.84708	0.000144	39.63
0:41:40	41.67	0.09696	8.90444	0.000136	39.61
0:42:25	42.42	0.09625	8.84273	0.000144	39.86
0:43:10	43.17	0.09549	9.00722	0.000123	40.30
0:43:55	43.92	0.09590	9.06457	0.000116	40.35
0:44:40	44.67	0.09604	9.04992	0.000117	40.29
0:45:25	45.42	0.09546	9.20671	0.000100	40.57
0:46:10	46.17	0.09491	9.09016	0.000113	40.42
0:46:55	46.92	0.09550	8.99602	0.000124	40.70
0:47:40	47.67	0.09482	8.96359	0.000128	41.02
0:48:25	48.42	0.09532	9.04045	0.000119	40.87

0:49:10	49.17	0.09452	8.96063	0.000128	41.03
0:49:55	49.92	0.09391	9.06141	0.000116	41.07
0:50:40	50.67	0.09424	9.13980	0.000107	41.15
0:51:25	51.42	0.09437	9.12867	0.000109	41.36
0:52:10	52.17	0.09470	9.14334	0.000107	41.28
0:52:55	52.92	0.09409	9.12489	0.000109	41.23
0:53:40	53.67	0.09478	9.08982	0.000113	41.29
0:54:25	54.42	0.09418	9.05270	0.000117	41.40
0:55:10	55.17	0.09456	8.87540	0.000140	41.38
0:55:55	55.92	0.09454	9.15037	0.000106	41.57
0:56:40	56.67	0.09376	9.03095	0.000120	41.81
0:57:25	57.42	0.09370	9.01143	0.000122	41.40
0:58:10	58.17	0.09387	8.82089	0.000148	41.62
0:58:55	58.92	0.09324	9.05311	0.000117	41.68
0:59:40	59.67	0.09375	9.03899	0.000119	41.87
1:00:25	60.42	0.09398	9.12726	0.000109	41.97
1:01:10	61.17	0.09410	9.16723	0.000104	41.74
1:01:55	61.92	0.09334	8.98936	0.000125	42.08
1:02:40	62.67	0.09349	8.94221	0.000131	41.59
1:03:25	63.42	0.09386	9.02005	0.000121	42.17
1:04:10	64.17	0.09402	9.00748	0.000122	41.89
1:04:55	64.92	0.09361	8.89568	0.000137	42.03
1:05:40	65.67	0.09310	9.05197	0.000117	42.40
1:06:25	66.42	0.09286	8.98066	0.000126	42.31
1:07:10	67.17	0.09355	8.96301	0.000128	42.46
1:07:55	67.92	0.09312	8.84986	0.000143	42.31
1:08:40	68.67	0.09347	8.97902	0.000126	42.36
1:09:25	69.42	0.09326	9.00814	0.000122	42.46
1:10:10	70.17	0.09292	9.00518	0.000123	42.49
1:10:55	70.92	0.09261	8.96896	0.000127	42.52
1:11:40	71.67	0.09255	8.94107	0.000131	42.62
1:12:25	72.42	0.09245	9.03401	0.000119	42.71
1:13:10	73.17	0.09357	8.92422	0.000133	42.69
1:13:55	73.92	0.09262	8.84554	0.000144	42.75
1:14:40	74.67	0.09273	8.86446	0.000141	42.81

1:15:25	75.42	0.09197	8.89743	0.000137	42.92
1:16:10	76.17	0.09257	8.85663	0.000142	43.06
1:16:55	76.92	0.09293	8.78498	0.000153	43.12
1:17:40	77.67	0.09147	8.71532	0.000164	43.03
1:18:25	78.42	0.09182	8.73015	0.000162	42.96
1:19:10	79.17	0.09255	8.73744	0.000160	43.17
1:19:55	79.92	0.09248	8.81568	0.000148	43.10
1:20:40	80.67	0.09212	8.82005	0.000148	43.19
1:21:25	81.42	0.09230	8.77711	0.000154	43.04
1:22:10	82.17	0.09237	8.70798	0.000165	43.27
1:22:55	82.92	0.09112	8.67255	0.000171	43.26
1:23:40	83.67	0.09076	8.56568	0.000191	43.36
1:24:25	84.42	0.09143	8.63894	0.000177	43.55
1:25:10	85.17	0.09176	8.71262	0.000164	43.45
1:25:55	85.92	0.09207	8.63265	0.000178	43.32
1:26:40	86.67	0.09143	8.63062	0.000179	43.37
1:27:25	87.42	0.09270	8.62707	0.000179	43.39
1:28:10	88.17	0.09151	8.54630	0.000194	43.34
1:28:55	88.92	0.09167	8.61604	0.000181	43.48
1:29:40	89.67	0.09190	8.67405	0.000171	43.60
1:30:25	90.42	0.09186	8.65176	0.000175	43.54
1:31:10	91.17	0.09145	8.63880	0.000177	43.42
1:31:55	91.92	0.09178	8.48175	0.000207	43.42
1:32:40	92.67	0.09142	8.48708	0.000206	43.68
1:33:25	93.42	0.09231	8.47410	0.000209	43.62
1:34:10	94.17	0.09294	8.50385	0.000203	43.60
1:34:55	94.92	0.09172	8.41927	0.000221	43.28
1:35:40	95.67	0.09187	8.54991	0.000194	43.55
1:36:25	96.42	0.09222	8.50686	0.000202	43.61
1:37:10	97.17	0.09179	8.47280	0.000209	43.76
1:37:55	97.92	0.09100	8.31513	0.000245	43.93
1:38:40	98.67	0.09092	8.38288	0.000229	43.63
1:39:25	99.42	0.09146	8.35212	0.000236	43.93
1:40:10	100.17	0.09172	8.41492	0.000222	43.66
1:40:55	100.92	0.09125	8.36702	0.000232	43.63

1:41:40	101.67	0.09166	8.43374	0.000217	43.70
1:42:25	102.42	0.09130	8.31532	0.000245	43.77
1:43:10	103.17	0.09103	8.36320	0.000233	43.91
1:43:55	103.92	0.09119	8.31805	0.000244	43.83
1:44:40	104.67	0.09060	8.37735	0.000230	43.89
1:45:25	105.42	0.09070	8.25189	0.000261	43.82
1:46:10	106.17	0.09103	8.33071	0.000241	43.87
1:46:55	106.92	0.09041	8.31713	0.000244	43.86
1:47:40	107.67	0.09041	8.38137	0.000229	43.65
1:48:25	108.42	0.09114	8.28230	0.000253	43.68
1:49:10	109.17	0.09091	8.24074	0.000264	43.77
1:49:55	109.92	0.09032	8.22851	0.000267	43.86
1:50:40	110.67	0.09063	8.23947	0.000264	43.85
1:51:25	111.42	0.09032	8.19141	0.000277	44.05
1:52:10	112.17	0.09010	8.20882	0.000272	43.93
1:52:55	112.92	0.09080	8.23252	0.000266	43.88
1:53:40	113.67	0.09108	8.23874	0.000264	43.77
1:54:25	114.42	0.09035	8.22661	0.000267	43.90
1:55:10	115.17	0.08999	8.29672	0.000249	43.87
1:55:55	115.92	0.09014	8.17422	0.000282	43.76
1:56:40	116.67	0.09006	8.22251	0.000269	44.03
1:57:25	117.42	0.09012	8.16146	0.000285	43.75
1:58:10	118.17	0.08975	8.20203	0.000274	44.12
1:58:55	118.92	0.08981	8.18248	0.000280	44.02
1:59:40	119.67	0.08963	8.16167	0.000285	43.97
2:00:25	120.42	0.08978	8.07428	0.000311	43.95
2:01:10	121.17	0.09020	8.04830	0.000320	43.95
2:01:55	121.92	0.08979	8.01753	0.000330	43.86
2:02:40	122.67	0.08967	8.03906	0.000323	43.88
2:03:25	123.42	0.08935	8.10521	0.000302	43.86
2:04:10	124.17	0.08946	8.13447	0.000293	43.93
2:04:55	124.92	0.08985	8.15171	0.000288	43.88
2:05:40	125.67	0.08972	8.22653	0.000267	43.79
2:06:25	126.42	0.09032	8.17221	0.000282	43.91
2:07:10	127.17	0.08967	8.12755	0.000295	43.98

2:07:55	127.92	0.08963	8.09287	0.000306	43.95
2:08:40	128.67	0.08953	8.12862	0.000295	43.91
2:09:25	129.42	0.09037	8.14827	0.000289	43.91
2:10:10	130.17	0.08911	8.15756	0.000287	43.80
2:10:55	130.92	0.09007	8.14585	0.000290	43.96
2:11:40	131.67	0.08976	8.15005	0.000289	43.95
2:12:25	132.42	0.08995	8.09307	0.000306	43.94
2:13:10	133.17	0.08890	8.10852	0.000301	43.97
2:13:55	133.92	0.08922	8.10509	0.000302	43.73
2:14:40	134.67	0.09009	8.12192	0.000297	44.04
2:15:25	135.42	0.08891	8.13699	0.000293	43.97
2:16:10	136.17	0.08947	8.04788	0.000320	44.02
2:16:55	136.92	0.08957	8.02563	0.000327	43.93
2:17:40	137.67	0.08847	8.08731	0.000307	44.07
2:18:25	138.42	0.08959	8.09584	0.000305	44.03
2:19:10	139.17	0.08879	8.03793	0.000323	43.93
2:19:55	139.92	0.08967	8.11724	0.000298	44.12
2:20:40	140.67	0.08901	8.04351	0.000321	43.93
2:21:25	141.42	0.08921	8.05074	0.000319	44.04
2:22:10	142.17	0.08878	8.01385	0.000331	43.98
2:22:55	142.92	0.08873	7.98817	0.000339	43.92
2:23:40	143.67	0.08935	7.96757	0.000347	43.84
2:24:25	144.42	0.08871	7.97442	0.000344	43.87
2:25:10	145.17	0.08917	7.99463	0.000337	43.84
2:25:55	145.92	0.08960	8.00431	0.000334	44.15
2:26:40	146.67	0.08907	8.00601	0.000333	43.89
2:27:25	147.42	0.08831	7.97161	0.000345	43.82
2:28:11	148.18	0.08927	7.95263	0.000352	44.07
2:28:55	148.92	0.08915	7.97386	0.000344	44.09
2:29:40	149.67	0.08874	8.03080	0.000325	44.03
2:30:25	150.42	0.08909	7.93404	0.000358	43.73
2:31:10	151.17	0.08808	7.94037	0.000356	43.90
2:31:56	151.93	0.08866	7.90923	0.000367	44.07
2:32:40	152.67	0.08841	7.90496	0.000369	44.08
2:33:25	153.42	0.08878	7.94623	0.000354	44.00

2:34:10	154.17	0.08907	7.93906	0.000357	43.83
2:34:55	154.92	0.08930	7.97276	0.000345	44.03
2:35:40	155.67	0.08876	7.97961	0.000342	44.01
2:36:25	156.42	0.08796	7.98153	0.000342	44.02
2:37:10	157.17	0.08819	7.95802	0.000350	43.95
2:37:55	157.92	0.08916	7.96851	0.000346	43.95
2:38:40	158.67	0.08837	7.95430	0.000351	44.02
2:39:25	159.42	0.08802	7.98833	0.000339	43.95
2:40:10	160.17	0.08930	7.91750	0.000364	44.12
2:40:55	160.92	0.08886	7.93029	0.000360	44.06
2:41:40	161.67	0.08870	7.91579	0.000365	43.90
2:42:25	162.42	0.08906	7.85393	0.000388	44.01
2:43:11	163.18	0.08767	7.89466	0.000373	43.93
2:43:55	163.92	0.08858	7.88081	0.000378	43.98
2:44:40	164.67	0.08828	7.84379	0.000392	43.93
2:45:26	165.43	0.08811	7.80323	0.000408	43.92
2:46:10	166.17	0.08795	7.84162	0.000393	43.86
2:46:56	166.93	0.08778	7.84247	0.000393	43.92
2:47:40	167.67	0.08797	7.82119	0.000401	44.12
2:48:25	168.42	0.08792	7.79832	0.000410	43.85
2:49:11	169.18	0.08735	7.80954	0.000406	43.92
2:49:55	169.92	0.08779	7.81780	0.000403	44.08
2:50:40	170.67	0.08860	7.81192	0.000405	44.04
2:51:25	171.42	0.08799	7.79656	0.000411	43.89
2:52:11	172.18	0.08810	7.83517	0.000396	44.03
2:52:56	172.93	0.08766	7.86136	0.000385	43.81
2:53:40	173.67	0.08786	7.83246	0.000397	43.84
2:54:25	174.42	0.08845	7.85019	0.000390	44.05
2:55:10	175.17	0.08836	7.80770	0.000407	43.88
2:55:55	175.92	0.08773	7.80558	0.000407	43.88
2:56:41	176.68	0.08785	7.81405	0.000404	43.90
2:57:25	177.42	0.08761	7.81905	0.000402	43.89
2:58:10	178.17	0.08775	7.77703	0.000419	43.83
2:58:55	178.92	0.08795	7.79962	0.000410	43.93
2:59:40	179.67	0.08764	7.77711	0.000419	43.89

3:00:26	180.43	0.08737	7.81037	0.000406	43.88
3:01:10	181.17	0.08810	7.77833	0.000419	44.01
3:01:56	181.93	0.08809	7.77389	0.000421	43.93
3:02:40	182.67	0.08809	7.77321	0.000421	43.81
3:03:25	183.42	0.08642	7.76819	0.000423	43.73
3:04:11	184.18	0.08782	7.74772	0.000432	43.91
3:04:55	184.92	0.08795	7.75219	0.000430	44.09
3:05:41	185.68	0.08689	7.73597	0.000437	43.84
3:06:25	186.42	0.08769	7.71884	0.000444	43.84
3:07:10	187.17	0.08688	7.70912	0.000449	43.89
3:07:56	187.93	0.08688	7.73297	0.000438	43.82
3:08:40	188.67	0.08700	7.74510	0.000433	43.92
3:09:25	189.42	0.08671	7.70652	0.000450	43.98
3:10:11	190.18	0.08672	7.68094	0.000462	43.88
3:10:55	190.92	0.08663	7.67272	0.000465	43.86
3:11:41	191.68	0.08650	7.63993	0.000481	43.67
3:12:25	192.42	0.08717	7.66563	0.000469	43.85
3:13:11	193.18	0.08688	7.69467	0.000455	44.13
3:13:56	193.93	0.08700	7.68080	0.000462	43.91
3:14:40	194.67	0.08713	7.66315	0.000470	43.90
3:15:26	195.43	0.08676	7.63073	0.000485	44.00
3:16:10	196.17	0.08757	7.67126	0.000466	43.97
3:16:56	196.93	0.08678	7.66194	0.000470	43.74
3:17:40	197.67	0.08637	7.58686	0.000507	43.85
3:18:26	198.43	0.08661	7.61004	0.000495	44.14
3:19:10	199.17	0.08578	7.61964	0.000491	43.82
3:19:56	199.93	0.08622	7.65174	0.000475	43.65
3:20:40	200.67	0.08618	7.64013	0.000481	43.85
3:21:26	201.43	0.08692	7.62298	0.000489	43.82
3:22:11	202.18	0.08634	7.62515	0.000488	44.04
3:22:55	202.92	0.08654	7.55215	0.000525	43.83
3:23:41	203.68	0.08628	7.55684	0.000523	43.80
3:24:25	204.42	0.08647	7.57332	0.000514	43.73
3:25:11	205.18	0.08658	7.53481	0.000534	43.89
3:25:55	205.92	0.08588	7.55015	0.000526	43.83

3:26:41	206.68	0.08607	7.54713	0.000528	43.88
3:27:25	207.42	0.08621	7.54873	0.000527	43.82
3:28:11	208.18	0.08571	7.58562	0.000508	43.75
3:28:56	208.93	0.08640	7.59549	0.000503	43.80
3:29:41	209.68	0.08553	7.55808	0.000522	43.83
3:30:26	210.43	0.08530	7.51815	0.000543	43.70
3:31:10	211.17	0.08572	7.50535	0.000550	43.75
3:31:56	211.93	0.08578	7.50478	0.000550	43.79
3:32:40	212.67	0.08502	7.54094	0.000531	43.92
3:33:26	213.43	0.08637	7.48908	0.000559	43.74
3:34:10	214.17	0.08542	7.55785	0.000522	43.99
3:34:56	214.93	0.08640	7.64487	0.000478	43.83
3:35:41	215.68	0.08599	7.70447	0.000451	43.78
3:36:25	216.42	0.08526	7.64636	0.000478	43.78
3:37:11	217.18	0.08665	7.62084	0.000490	43.76
3:37:55	217.92	0.08557	7.59910	0.000501	43.73
3:38:41	218.68	0.08539	7.58350	0.000509	43.70
3:39:25	219.42	0.08562	7.57245	0.000514	43.62
3:40:11	220.18	0.08557	7.55532	0.000523	43.76
3:40:56	220.93	0.08535	7.54786	0.000527	43.92
3:41:41	221.68	0.08536	7.53681	0.000533	44.01
3:42:26	222.43	0.08521	7.54495	0.000529	43.70
3:43:10	223.17	0.08560	7.51469	0.000545	43.76
3:43:56	223.93	0.08565	7.47945	0.000565	43.74
3:44:40	224.67	0.08609	7.48719	0.000560	43.78
3:45:26	225.43	0.08546	7.47215	0.000569	43.88
3:46:11	226.18	0.08485	7.44944	0.000582	43.80
3:46:55	226.92	0.08451	7.45497	0.000579	43.65
3:47:41	227.68	0.08410	7.44047	0.000587	43.63
3:48:25	228.42	0.08480	7.44189	0.000586	43.91
3:49:11	229.18	0.08444	7.43623	0.000590	43.73
3:49:56	229.93	0.08382	7.40992	0.000605	43.89
3:50:41	230.68	0.08431	7.39597	0.000614	43.68
3:51:26	231.43	0.08417	7.40341	0.000609	43.65
3:52:10	232.17	0.08451	7.42168	0.000598	43.62

3:52:56	232.93	0.08444	7.40159	0.000610	43.62
3:53:40	233.67	0.08486	7.38376	0.000621	43.59
3:54:26	234.43	0.08377	7.39081	0.000617	43.74
3:55:11	235.18	0.08388	7.37982	0.000624	44.06
3:55:55	235.92	0.08477	7.38944	0.000618	43.58
3:56:41	236.68	0.08353	7.37830	0.000625	43.84
3:57:25	237.42	0.08409	7.36104	0.000636	43.78
3:58:11	238.18	0.08385	7.35784	0.000638	43.91
3:58:56	238.93	0.08442	7.34630	0.000645	43.52
3:59:41	239.68	0.08365	7.34955	0.000643	43.67
4:00:26	240.43	0.08291	7.33407	0.000653	43.52
4:01:10	241.17	0.08342	7.29847	0.000677	43.92
4:01:56	241.93	0.08342	7.31670	0.000664	43.58
4:02:40	242.67	0.08353	7.30171	0.000674	43.75
4:03:26	243.43	0.08333	7.30096	0.000675	43.73
4:04:11	244.18	0.08363	7.29395	0.000680	43.70
4:04:56	244.93	0.08426	7.29926	0.000676	43.71
4:05:41	245.68	0.08397	7.29552	0.000679	43.83
4:06:26	246.43	0.08359	7.27541	0.000692	43.72
4:07:11	247.18	0.08244	7.27445	0.000693	43.69
4:07:56	247.93	0.08287	7.26853	0.000697	43.67
4:08:41	248.68	0.08344	7.24609	0.000713	43.61
4:09:26	249.43	0.08343	7.26042	0.000703	43.73
4:10:11	250.18	0.08315	7.25022	0.000710	43.78
4:10:56	250.93	0.08304	7.24375	0.000715	43.53
4:11:41	251.68	0.08239	7.22328	0.000729	43.55
4:12:26	252.43	0.08306	7.23949	0.000718	43.65
4:13:11	253.18	0.08237	7.22431	0.000729	43.71
4:13:56	253.93	0.08217	7.19764	0.000748	43.81
4:14:41	254.68	0.08230	7.24506	0.000714	43.63
4:15:25	255.42	0.08323	7.23986	0.000717	43.84
4:16:11	256.18	0.08284	7.19214	0.000752	43.71
4:16:56	256.93	0.08264	7.19933	0.000747	43.64
4:17:41	257.68	0.08251	7.22947	0.000725	43.48
4:18:26	258.43	0.08218	7.24021	0.000717	43.68

4:19:10	259.17	0.08283	7.23510	0.000721	43.56
4:19:56	259.93	0.08286	7.21382	0.000736	43.87
4:20:41	260.68	0.08212	7.22749	0.000726	43.65
4:21:26	261.43	0.08298	7.21054	0.000739	43.54
4:22:11	262.18	0.08251	7.20987	0.000739	43.55
4:22:55	262.92	0.08246	7.22774	0.000726	43.76
4:23:41	263.68	0.08142	7.20520	0.000743	43.59
4:24:26	264.43	0.08220	7.24247	0.000716	43.61
4:25:11	265.18	0.08253	7.24645	0.000713	43.53
4:25:56	265.93	0.08254	7.21187	0.000738	43.60
4:26:41	266.68	0.08188	7.22132	0.000731	43.58
4:27:26	267.43	0.08265	7.20534	0.000743	43.45
4:28:11	268.18	0.08191	7.22895	0.000725	43.58
4:28:56	268.93	0.08287	7.21342	0.000737	43.56
4:29:41	269.68	0.08351	7.21087	0.000739	43.42
4:30:26	270.43	0.08294	7.20451	0.000743	43.74
4:31:11	271.18	0.08251	7.23239	0.000723	43.67
4:31:56	271.93	0.08282	7.17233	0.000768	43.54
4:32:41	272.68	0.08252	7.17920	0.000762	43.72
4:33:26	273.43	0.08238	7.15732	0.000779	43.59
4:34:11	274.18	0.08155	7.16713	0.000772	43.57
4:34:56	274.93	0.08190	7.14576	0.000788	43.63
4:35:41	275.68	0.08249	7.15908	0.000778	43.64
4:36:26	276.43	0.08196	7.14821	0.000786	43.56
4:37:11	277.18	0.08216	7.15085	0.000784	43.51
4:37:56	277.93	0.08160	7.14753	0.000787	43.28
4:38:41	278.68	0.08099	7.15312	0.000782	43.57
4:39:26	279.43	0.08188	7.13076	0.000800	43.60
4:40:11	280.18	0.08218	7.11703	0.000811	43.57
4:40:56	280.93	0.08232	7.10930	0.000817	43.78
4:41:41	281.68	0.08115	7.11558	0.000812	43.56
4:42:26	282.43	0.08166	7.11531	0.000813	43.60
4:43:11	283.18	0.08083	7.13415	0.000797	43.69
4:43:56	283.93	0.08129	7.10241	0.000823	43.57
4:44:41	284.68	0.08192	7.11396	0.000814	43.54

4:45:26	285.43	0.08136	7.15151	0.000784	43.62
4:46:11	286.18	0.08148	7.15925	0.000778	43.59
4:46:56	286.93	0.08102	7.14003	0.000793	43.49
4:47:41	287.68	0.08069	7.11802	0.000810	43.69
4:48:26	288.43	0.08057	7.12017	0.000809	43.59
4:49:11	289.18	0.07986	7.10603	0.000820	43.64
4:49:56	289.93	0.08075	7.08987	0.000834	43.60
4:50:41	290.68	0.08048	7.09769	0.000827	43.60
4:51:26	291.43	0.08048	7.09739	0.000827	43.54
4:52:11	292.18	0.08095	7.08169	0.000840	43.64
4:52:56	292.93	0.08033	7.08976	0.000834	43.73
4:53:41	293.68	0.07947	7.09888	0.000826	43.44
4:54:26	294.43	0.08065	7.06058	0.000858	43.70
4:55:11	295.18	0.08033	7.06693	0.000853	43.59
4:55:56	295.93	0.08064	7.06907	0.000851	43.52
4:56:41	296.68	0.08137	7.06423	0.000855	43.54
4:57:26	297.43	0.08017	7.05096	0.000867	43.54
4:58:11	298.18	0.07973	7.07131	0.000849	43.52
4:58:56	298.93	0.08047	7.08906	0.000834	43.54
4:59:41	299.68	0.08061	7.05789	0.000861	43.44
5:00:26	300.43	0.08060	7.07074	0.000850	43.58
5:01:11	301.18	0.08071	7.07095	0.000849	43.51
5:01:56	301.93	0.08004	7.05742	0.000861	43.45
5:02:41	302.68	0.08031	7.06892	0.000851	43.54
5:03:26	303.43	0.07899	7.06257	0.000857	43.43
5:04:11	304.18	0.08026	7.06245	0.000857	43.60
5:04:56	304.93	0.08013	7.05942	0.000859	43.45
5:05:41	305.68	0.07983	7.04056	0.000876	43.48
5:06:26	306.43	0.08027	7.04623	0.000871	43.44
5:07:11	307.18	0.07963	7.02048	0.000893	43.49
5:07:56	307.93	0.07998	7.04636	0.000871	43.57
5:08:41	308.68	0.08011	7.04024	0.000876	43.48
5:09:26	309.43	0.08040	7.01415	0.000899	43.46
5:10:11	310.18	0.07929	7.02707	0.000888	43.54
5:10:56	310.93	0.08031	7.01716	0.000896	43.48

5:11:41	311.68	0.08012	6.99962	0.000912	43.48
5:12:26	312.43	0.07983	7.03104	0.000884	43.40
5:13:11	313.18	0.07890	7.01262	0.000900	43.39
5:13:56	313.93	0.07927	7.00384	0.000908	43.37
5:14:41	314.68	0.07960	7.00709	0.000905	43.41
5:15:26	315.43	0.07914	6.98628	0.000924	43.49
5:16:11	316.18	0.07840	6.97551	0.000934	43.52
5:16:56	316.93	0.07868	6.97964	0.000931	43.65
5:17:41	317.68	0.07891	6.99380	0.000918	43.46
5:18:26	318.43	0.07837	6.98378	0.000927	43.46
5:19:11	319.18	0.07920	6.95120	0.000957	43.45
5:19:56	319.93	0.07827	6.96126	0.000948	43.41
5:20:41	320.68	0.07901	6.94700	0.000962	43.42
5:21:26	321.43	0.07886	6.96669	0.000943	43.46
5:22:11	322.18	0.07867	6.96568	0.000944	43.30
5:22:56	322.93	0.07874	6.95590	0.000953	43.43
5:23:41	323.68	0.07889	6.94151	0.000967	43.45
5:24:26	324.43	0.07835	6.92886	0.000979	43.57
5:25:11	325.18	0.07811	6.90885	0.000999	43.49
5:25:56	325.93	0.07886	6.90467	0.001003	43.33
5:26:41	326.68	0.07833	6.93275	0.000975	43.36
5:27:26	327.43	0.07849	6.96269	0.000947	43.35
5:28:11	328.18	0.07812	6.94100	0.000967	43.30
5:28:56	328.93	0.07840	6.94509	0.000963	43.37
5:29:41	329.68	0.07841	6.93435	0.000974	43.48
5:30:26	330.43	0.07838	6.92340	0.000984	43.40
5:31:10	331.17	0.07829	6.92867	0.000979	43.28
5:31:56	331.93	0.07815	6.90959	0.000998	43.33
5:32:41	332.68	0.07820	6.91804	0.000990	43.32
5:33:25	333.42	0.07767	6.94339	0.000965	43.39
5:34:11	334.18	0.07756	6.91453	0.000993	43.13
5:34:55	334.92	0.07807	6.92522	0.000983	43.54
5:35:40	335.67	0.07807	6.90941	0.000998	43.40
5:36:26	336.43	0.07723	6.88600	0.001022	43.11
5:37:11	337.18	0.07804	6.89193	0.001016	43.34

5:37:55	337.92	0.07799	6.89404	0.001014	43.35
5:38:41	338.68	0.07756	6.88855	0.001019	43.30
5:39:26	339.43	0.07741	6.89108	0.001017	43.32
5:40:11	340.18	0.07789	6.90487	0.001003	43.36
5:40:55	340.92	0.07752	6.89662	0.001011	43.26
5:41:41	341.68	0.07765	6.89082	0.001017	43.24
5:42:26	342.43	0.07748	6.88603	0.001022	43.18
5:43:11	343.18	0.07827	6.88600	0.001022	43.33
5:43:56	343.93	0.07798	6.89747	0.001010	43.44
5:44:41	344.68	0.07684	6.88162	0.001026	43.31
5:45:25	345.42	0.07810	6.88192	0.001026	43.32
5:46:11	346.18	0.07716	6.86104	0.001048	43.27
5:46:56	346.93	0.07743	6.85750	0.001052	43.52
5:47:41	347.68	0.07675	6.87849	0.001030	43.12
5:48:26	348.43	0.07666	6.87298	0.001035	43.32
5:49:11	349.18	0.07700	6.88440	0.001024	43.36
5:49:56	349.93	0.07711	6.88882	0.001019	43.15
5:50:41	350.68	0.07684	6.86517	0.001044	43.35
5:51:26	351.43	0.07678	6.86352	0.001045	43.29
5:52:11	352.18	0.07661	6.86594	0.001043	43.26
5:52:56	352.93	0.07696	6.85722	0.001052	43.19
5:53:41	353.68	0.07608	6.86755	0.001041	43.32
5:54:26	354.43	0.07730	6.86804	0.001041	43.29
5:55:11	355.18	0.07661	6.84557	0.001064	43.40
5:55:56	355.93	0.07701	6.86975	0.001039	43.61
5:56:41	356.68	0.07674	6.86096	0.001048	43.56
5:57:26	357.43	0.07681	6.87382	0.001035	43.28
5:58:11	358.18	0.07645	6.84571	0.001064	43.48
5:58:56	358.93	0.07622	6.86164	0.001047	43.32
5:59:41	359.68	0.07691	6.84914	0.001060	43.48
6:00:26	360.43	0.07689	6.85805	0.001051	43.24
6:01:11	361.18	0.07633	6.85818	0.001051	43.19
6:01:56	361.93	0.07651	6.86688	0.001042	43.31
6:02:41	362.68	0.07669	6.88044	0.001028	43.41
6:03:26	363.43	0.07618	6.85772	0.001051	43.30

6:04:11	364.18	0.07605	6.84581	0.001064	43.52
6:04:56	364.93	0.07645	6.83621	0.001074	43.37
6:05:41	365.68	0.07587	6.83820	0.001072	43.37
6:06:26	366.43	0.07634	6.86162	0.001047	43.38
6:07:11	367.18	0.07587	6.83918	0.001071	43.25
6:07:56	367.93	0.07616	6.81645	0.001096	43.22
6:08:41	368.68	0.07527	6.82196	0.001090	43.35
6:09:26	369.43	0.07471	6.80791	0.001105	43.34
6:10:11	370.18	0.07646	6.83025	0.001081	43.35
6:10:56	370.93	0.07619	6.83251	0.001078	43.40
6:11:41	371.68	0.07507	6.79976	0.001114	43.46
6:12:26	372.43	0.07526	6.79782	0.001116	43.38
6:13:11	373.18	0.07504	6.80517	0.001108	43.10
6:13:56	373.93	0.07515	6.81504	0.001097	43.21
6:14:41	374.68	0.07558	6.80149	0.001112	43.40
6:15:26	375.43	0.07559	6.81097	0.001102	43.43
6:16:11	376.18	0.07517	6.80950	0.001103	43.33
6:16:56	376.93	0.07523	6.78402	0.001132	43.15
6:17:41	377.68	0.07550	6.78423	0.001131	43.26
6:18:26	378.43	0.07561	6.79802	0.001116	43.20
6:19:11	379.18	0.07497	6.78933	0.001126	43.33
6:19:56	379.93	0.07451	6.78309	0.001133	43.29
6:20:41	380.68	0.07408	6.76423	0.001154	43.37
6:21:26	381.43	0.07462	6.76107	0.001158	43.22
6:22:11	382.18	0.07483	6.76596	0.001152	43.26
6:22:56	382.93	0.07502	6.78758	0.001128	43.12
6:23:41	383.68	0.07447	6.76213	0.001157	43.42
6:24:26	384.43	0.07454	6.75864	0.001161	43.31
6:25:11	385.18	0.07353	6.74700	0.001174	43.06
6:25:56	385.93	0.07408	6.75227	0.001168	43.18
6:26:41	386.68	0.07414	6.75404	0.001166	43.16
6:27:26	387.43	0.07509	6.76703	0.001151	43.40
6:28:11	388.18	0.07549	6.76730	0.001151	43.21
6:28:56	388.93	0.07436	6.73438	0.001189	43.26
6:29:41	389.68	0.07448	6.75156	0.001169	43.04

6:30:26	390.43	0.07388	6.74920	0.001172	43.34
6:31:11	391.18	0.07407	6.73731	0.001186	43.19
6:31:56	391.93	0.07389	6.74940	0.001172	43.21
6:32:41	392.68	0.07441	6.76454	0.001154	43.20
6:33:26	393.43	0.07378	6.75316	0.001167	43.43
6:34:11	394.18	0.07470	6.73826	0.001185	43.23
6:34:56	394.93	0.07387	6.73086	0.001194	43.38
6:35:41	395.68	0.07347	6.71570	0.001212	43.24
6:36:26	396.43	0.07339	6.71727	0.001210	43.03
6:37:11	397.18	0.07321	6.69647	0.001235	43.18
6:37:56	397.93	0.07305	6.68549	0.001249	43.17
6:38:41	398.68	0.07354	6.68816	0.001246	43.17
6:39:26	399.43	0.07287	6.68353	0.001251	43.17
6:40:11	400.18	0.07293	6.66963	0.001269	43.15
6:40:56	400.93	0.07294	6.69620	0.001236	43.21
6:41:41	401.68	0.07283	6.70463	0.001225	43.08
6:42:26	402.43	0.07304	6.68657	0.001248	43.30
6:43:11	403.18	0.07332	6.68400	0.001251	43.23
6:43:56	403.93	0.07266	6.70767	0.001222	43.09
6:44:41	404.68	0.07274	6.70166	0.001229	43.23
6:45:26	405.43	0.07225	6.66836	0.001270	43.05
6:46:11	406.18	0.07255	6.67617	0.001261	43.42
6:46:56	406.93	0.07247	6.66589	0.001274	43.05
6:47:41	407.68	0.07262	6.65088	0.001293	43.09
6:48:26	408.43	0.07237	6.64738	0.001297	43.20
6:49:11	409.18	0.07218	6.64749	0.001297	43.12
6:49:56	409.93	0.07219	6.65526	0.001287	43.19
6:50:41	410.68	0.07217	6.65451	0.001288	43.32
6:51:26	411.43	0.07189	6.65354	0.001289	43.24
6:52:11	412.18	0.07186	6.65295	0.001290	43.15
6:52:56	412.93	0.07223	6.63689	0.001311	43.19
6:53:41	413.68	0.07124	6.62905	0.001321	42.92
6:54:26	414.43	0.07178	6.63719	0.001311	43.14
6:55:11	415.18	0.07194	6.62960	0.001321	43.16
6:55:56	415.93	0.07220	6.61837	0.001336	43.04

6:56:41	416.68	0.07211	6.62375	0.001328	43.18
6:57:26	417.43	0.07145	6.61311	0.001343	42.96
6:58:11	418.18	0.07167	6.61502	0.001340	43.17
6:58:56	418.93	0.07104	6.62040	0.001333	43.07
6:59:41	419.68	0.07182	6.60352	0.001356	43.27
7:00:26	420.43	0.07148	6.61024	0.001347	43.05
7:01:11	421.18	0.07071	6.59620	0.001366	43.03
7:01:56	421.93	0.07238	6.61385	0.001342	43.16
7:02:41	422.68	0.07136	6.60123	0.001359	43.10
7:03:26	423.43	0.07154	6.59871	0.001362	43.11
7:04:11	424.18	0.07138	6.58251	0.001384	43.22
7:04:56	424.93	0.07125	6.60724	0.001351	43.05
7:05:41	425.68	0.07104	6.61534	0.001340	43.01
7:06:26	426.43	0.07126	6.62642	0.001325	42.91
7:07:11	427.18	0.07198	6.62516	0.001327	42.94
7:07:56	427.93	0.07122	6.63337	0.001316	43.13
7:08:41	428.68	0.07148	6.61672	0.001338	43.06
7:09:26	429.43	0.07149	6.61194	0.001344	43.04
7:10:11	430.18	0.07148	6.61448	0.001341	43.10
7:10:56	430.93	0.07118	6.62222	0.001330	43.20
7:11:41	431.68	0.07201	6.62946	0.001321	43.11
7:12:26	432.43	0.07178	6.62914	0.001321	43.16
7:13:11	433.18	0.07217	6.62442	0.001328	43.02
7:13:56	433.93	0.07170	6.63481	0.001314	42.85
7:14:41	434.68	0.07276	6.63997	0.001307	43.23
7:15:26	435.43	0.07167	6.63118	0.001319	42.93
7:16:11	436.18	0.07228	6.64828	0.001296	42.86
7:16:56	436.93	0.07271	6.64737	0.001297	43.03
7:17:41	437.68	0.07249	6.65950	0.001282	43.09
7:18:26	438.43	0.07242	6.66488	0.001275	43.11
7:19:11	439.18	0.07257	6.66480	0.001275	43.03
7:19:57	439.95	0.07237	6.65959	0.001282	43.07
7:20:41	440.68	0.07195	6.65587	0.001286	43.03
7:21:26	441.43	0.07249	6.67744	0.001259	42.99
7:22:11	442.18	0.07256	6.67641	0.001260	43.18

7:22:56	442.93	0.07263	6.67349	0.001264	43.06
7:23:41	443.68	0.07258	6.68405	0.001251	43.20
7:24:26	444.43	0.07288	6.67828	0.001258	43.24
7:25:11	445.18	0.07132	6.66185	0.001279	43.16
7:25:57	445.95	0.07320	6.68123	0.001254	43.22
7:26:41	446.68	0.07234	6.69952	0.001231	43.14
7:27:26	447.43	0.07238	6.67917	0.001257	43.41
7:28:12	448.20	0.07256	6.66719	0.001272	43.21
7:28:56	448.93	0.07177	6.66100	0.001280	43.11
7:29:41	449.68	0.07230	6.67685	0.001260	43.17
7:30:26	450.43	0.07198	6.65497	0.001288	42.95
7:31:11	451.18	0.07203	6.67024	0.001268	42.89
7:31:56	451.93	0.07173	6.67342	0.001264	43.06
7:32:41	452.68	0.07148	6.67192	0.001266	42.95
7:33:26	453.43	0.07149	6.67120	0.001267	43.04
7:34:12	454.20	0.07162	6.67087	0.001267	43.18
7:34:56	454.93	0.07253	6.66924	0.001269	43.09
7:35:41	455.68	0.07227	6.65881	0.001283	43.17
7:36:27	456.45	0.07220	6.64648	0.001299	42.93
7:37:11	457.18	0.07192	6.64032	0.001307	42.96
7:37:56	457.93	0.07086	6.63860	0.001309	42.87
7:38:41	458.68	0.07193	6.63755	0.001310	43.06
7:39:26	459.43	0.07209	6.65349	0.001290	43.06
7:40:12	460.20	0.07168	6.63993	0.001307	43.08
7:40:56	460.93	0.07098	6.64668	0.001298	43.08
7:41:41	461.68	0.07224	6.66075	0.001280	43.23
7:42:27	462.45	0.07143	6.66178	0.001279	42.95
7:43:11	463.18	0.07188	6.64862	0.001296	43.20
7:43:57	463.95	0.07212	6.65384	0.001289	43.24
7:44:41	464.68	0.07141	6.65119	0.001292	43.07
7:45:26	465.43	0.07053	6.63032	0.001320	43.09
7:46:12	466.20	0.07116	6.64059	0.001306	43.07
7:46:56	466.93	0.07193	6.65413	0.001289	43.06
7:47:41	467.68	0.07151	6.65070	0.001293	43.11
7:48:27	468.45	0.07208	6.68565	0.001249	43.04

7:49:11	469.18	0.07218	6.67298	0.001265	43.01
7:49:57	469.95	0.07223	6.65945	0.001282	42.93
7:50:41	470.68	0.07151	6.66413	0.001276	42.96
7:51:26	471.43	0.07199	6.66246	0.001278	42.93
7:52:12	472.20	0.07177	6.67125	0.001267	43.01
7:52:56	472.93	0.07172	6.65444	0.001288	43.04
7:53:41	473.68	0.07202	6.66521	0.001274	43.10
7:54:27	474.45	0.07225	6.67234	0.001265	43.15
7:55:11	475.18	0.07099	6.67156	0.001266	43.08
7:55:56	475.93	0.07124	6.65056	0.001293	43.01
7:56:42	476.70	0.07109	6.66496	0.001275	43.11
7:57:26	477.43	0.07109	6.65893	0.001283	42.93
7:58:12	478.20	0.07133	6.64669	0.001298	43.01
7:58:56	478.93	0.07136	6.64592	0.001299	43.03
7:59:41	479.68	0.07110	6.64476	0.001301	43.23
8:00:27	480.45	0.07124	6.64510	0.001300	42.88
8:01:11	481.18	0.07232	6.63792	0.001310	43.07
8:01:57	481.95	0.07119	6.61891	0.001335	42.96
8:02:41	482.68	0.07037	6.62899	0.001321	43.21
8:03:26	483.43	0.07085	6.62572	0.001326	43.12
8:04:12	484.20	0.07000	6.63149	0.001318	43.04
8:04:56	484.93	0.07038	6.61807	0.001336	43.15
8:05:42	485.70	0.07014	6.62025	0.001333	42.94
8:06:27	486.45	0.06924	6.59534	0.001367	42.94
8:07:11	487.18	0.07049	6.60502	0.001354	43.11
8:07:57	487.95	0.07084	6.61338	0.001342	42.91
8:08:41	488.68	0.07045	6.60214	0.001357	43.04
8:09:27	489.45	0.06955	6.60437	0.001354	42.92
8:10:12	490.20	0.06899	6.59050	0.001373	42.88
8:10:56	490.93	0.06984	6.58614	0.001379	42.83
8:11:42	491.70	0.07064	6.57748	0.001391	43.03
8:12:26	492.43	0.06968	6.57370	0.001397	42.93
8:13:12	493.20	0.07021	6.58640	0.001379	42.89
8:13:57	493.95	0.06917	6.57186	0.001399	42.88
8:14:41	494.68	0.06887	6.55814	0.001419	43.05

8:15:27	495.45	0.06920	6.55468	0.001423	42.86
8:16:11	496.18	0.06882	6.55331	0.001425	42.83
8:16:56	496.93	0.06933	6.55156	0.001428	42.96
8:17:42	497.70	0.06856	6.54402	0.001439	42.85
8:18:26	498.43	0.06929	6.54801	0.001433	43.18
8:19:12	499.20	0.06869	6.53694	0.001449	42.98
8:19:57	499.95	0.06903	6.54603	0.001436	42.98
8:20:42	500.70	0.06833	6.54470	0.001438	43.07
8:21:27	501.45	0.06919	6.54228	0.001441	43.03
8:22:11	502.18	0.06909	6.51993	0.001474	42.99
8:22:57	502.95	0.06879	6.52870	0.001461	42.90
8:23:42	503.70	0.06861	6.53102	0.001458	42.70
8:24:26	504.43	0.06838	6.53821	0.001447	42.72
8:25:12	505.20	0.06924	6.52993	0.001459	42.99
8:25:56	505.93	0.06968	6.54051	0.001444	43.00
8:26:42	506.70	0.06847	6.53720	0.001449	43.09
8:27:27	507.45	0.06879	6.53615	0.001450	43.07
8:28:11	508.18	0.06762	6.53307	0.001455	43.13
8:28:57	508.95	0.06844	6.51351	0.001483	42.71
8:29:41	509.68	0.06737	6.50657	0.001494	43.00
8:30:27	510.45	0.06814	6.50529	0.001496	42.88
8:31:12	511.20	0.06793	6.52025	0.001473	43.04
8:31:56	511.93	0.06825	6.49381	0.001513	42.97
8:32:42	512.70	0.06790	6.49907	0.001505	43.03
8:33:26	513.43	0.06783	6.49574	0.001510	42.90
8:34:12	514.20	0.06815	6.49689	0.001508	42.92
8:34:57	514.95	0.06749	6.49034	0.001518	42.97
8:35:41	515.68	0.06697	6.48149	0.001532	42.91
8:36:27	516.45	0.06715	6.48562	0.001525	42.93
8:37:11	517.18	0.06710	6.47011	0.001549	42.89
8:37:57	517.95	0.06700	6.47480	0.001542	42.80
8:38:43	518.72	0.06657	6.45479	0.001573	42.89
8:39:28	519.47	0.06720	6.44999	0.001581	43.01
8:40:13	520.22	0.06680	6.44582	0.001587	42.80
8:40:58	520.97	0.06688	6.43090	0.001611	43.11

8:41:43	521.72	0.06611	6.45636	0.001571	43.03
8:42:28	522.47	0.06647	6.43987	0.001597	42.92
8:43:13	523.22	0.06523	6.43974	0.001597	42.80
8:43:57	523.95	0.06650	6.43606	0.001603	42.93
8:44:42	524.70	0.06567	6.44909	0.001582	42.92
8:45:27	525.45	0.06603	6.44826	0.001583	42.83
8:46:12	526.20	0.06579	6.42761	0.001616	42.68
8:46:57	526.95	0.06608	6.42696	0.001617	42.87
8:47:42	527.70	0.06576	6.41457	0.001638	42.85
8:48:27	528.45	0.06593	6.42685	0.001618	42.81
8:49:12	529.20	0.06509	6.41389	0.001639	42.95
8:49:57	529.95	0.06515	6.40354	0.001656	42.91
8:50:42	530.70	0.06528	6.40325	0.001656	42.78
8:51:27	531.45	0.06545	6.41879	0.001631	42.82
8:52:12	532.20	0.06567	6.39456	0.001671	42.93
8:52:57	532.95	0.06523	6.40238	0.001658	42.87
8:53:42	533.70	0.06533	6.40201	0.001658	42.66
8:54:27	534.45	0.06565	6.39183	0.001675	42.75
8:55:12	535.20	0.06451	6.37645	0.001701	42.87
8:55:57	535.95	0.06494	6.38584	0.001685	42.87
8:56:42	536.70	0.06496	6.37528	0.001703	42.89
8:57:27	537.45	0.06457	6.36956	0.001713	42.84
8:58:12	538.20	0.06446	6.35636	0.001736	42.71
8:58:57	538.95	0.06403	6.37514	0.001703	42.86
8:59:42	539.70	0.06403	6.36437	0.001722	42.79
9:00:27	540.45	0.06446	6.35995	0.001729	42.79
9:01:12	541.20	0.06402	6.36661	0.001718	42.76
9:01:57	541.95	0.06419	6.36021	0.001729	42.97
9:02:42	542.70	0.06403	6.35996	0.001729	42.67
9:03:27	543.45	0.06354	6.35760	0.001734	42.57
9:04:12	544.20	0.06403	6.36073	0.001728	42.85
9:04:57	544.95	0.06376	6.36586	0.001719	42.69
9:05:42	545.70	0.06418	6.36140	0.001727	42.76
9:06:27	546.45	0.06457	6.35903	0.001731	42.66
9:07:12	547.20	0.06449	6.37172	0.001709	42.77

9:07:57	547.95	0.06472	6.35079	0.001745	42.71
9:08:42	548.70	0.06384	6.36370	0.001723	42.67
9:09:27	549.45	0.06358	6.36211	0.001726	42.74
9:10:12	550.20	0.06369	6.36691	0.001717	42.49
9:10:57	550.95	0.06353	6.34866	0.001749	42.77
9:11:42	551.70	0.06342	6.34819	0.001750	42.50
9:12:27	552.45	0.06460	6.34559	0.001754	42.46
9:13:12	553.20	0.06330	6.33401	0.001775	42.66
9:13:57	553.95	0.06359	6.34522	0.001755	42.79
9:14:42	554.70	0.06389	6.34726	0.001752	42.71
9:15:27	555.45	0.06331	6.33233	0.001778	42.85
9:16:12	556.20	0.06333	6.32978	0.001782	42.76
9:16:57	556.95	0.06249	6.32555	0.001790	42.70
9:17:42	557.70	0.06305	6.32969	0.001783	42.59
9:18:27	558.45	0.06353	6.32226	0.001796	42.63
9:19:12	559.20	0.06248	6.31058	0.001817	42.81
9:19:57	559.95	0.06239	6.30596	0.001825	42.84
9:20:42	560.70	0.06381	6.31252	0.001813	42.76
9:21:27	561.45	0.06274	6.29589	0.001844	42.57
9:22:12	562.20	0.06262	6.30059	0.001835	42.78
9:22:57	562.95	0.06229	6.29181	0.001851	42.50
9:23:42	563.70	0.06282	6.30536	0.001826	42.69
9:24:27	564.45	0.06235	6.29714	0.001842	42.64
9:25:12	565.20	0.06179	6.29920	0.001838	42.56
9:25:57	565.95	0.06164	6.27842	0.001876	42.70
9:26:42	566.70	0.06113	6.28157	0.001870	42.66
9:27:27	567.45	0.06149	6.27652	0.001880	42.71
9:28:12	568.20	0.06171	6.28167	0.001870	42.55
9:28:57	568.95	0.06213	6.26939	0.001893	42.60
9:29:42	569.70	0.06203	6.27723	0.001879	42.54
9:30:27	570.45	0.06129	6.26445	0.001903	42.86
9:31:12	571.20	0.06118	6.26812	0.001896	42.55
9:31:57	571.95	0.06107	6.24949	0.001931	42.58
9:32:42	572.70	0.06086	6.24775	0.001935	42.71
9:33:27	573.45	0.06042	6.24688	0.001936	42.72

9:34:12	574.20	0.06046	6.23622	0.001957	42.63
9:34:57	574.95	0.06042	6.23705	0.001956	42.60
9:35:42	575.70	0.06043	6.23151	0.001966	42.48
9:36:27	576.45	0.06069	6.24033	0.001949	42.60
9:37:12	577.20	0.06010	6.22760	0.001974	42.54
9:37:57	577.95	0.05990	6.22900	0.001971	42.81
9:38:42	578.70	0.05999	6.22981	0.001970	42.59
9:39:27	579.45	0.05999	6.21293	0.002003	42.55
9:40:12	580.20	0.05970	6.21244	0.002004	42.55
9:40:57	580.95	0.06018	6.21251	0.002004	42.58
9:41:42	581.70	0.05924	6.21644	0.001996	42.54
9:42:27	582.45	0.06065	6.21848	0.001992	42.38
9:43:12	583.20	0.05935	6.21243	0.002004	42.43
9:43:57	583.95	0.05976	6.21234	0.002005	42.44
9:44:42	584.70	0.06042	6.20788	0.002013	42.49
9:45:27	585.45	0.05908	6.20798	0.002013	42.58
9:46:12	586.20	0.05959	6.20384	0.002022	42.79
9:46:57	586.95	0.05885	6.19767	0.002034	42.49
9:47:42	587.70	0.05861	6.20278	0.002024	42.55
9:48:27	588.45	0.05927	6.21026	0.002009	42.44
9:49:12	589.20	0.05958	6.20046	0.002029	42.49
9:49:57	589.95	0.05902	6.18810	0.002054	42.44
9:50:42	590.70	0.05828	6.18375	0.002063	42.46
9:51:27	591.45	0.05836	6.19030	0.002049	42.56
9:52:12	592.20	0.05861	6.18732	0.002055	42.35
9:52:57	592.95	0.05865	6.18594	0.002058	42.58
9:53:42	593.70	0.05826	6.18549	0.002059	42.66
9:54:27	594.45	0.05797	6.18240	0.002065	42.43
9:55:12	595.20	0.05887	6.18748	0.002055	42.30
9:55:57	595.95	0.05830	6.17928	0.002072	42.53
9:56:42	596.70	0.05824	6.17570	0.002079	42.33
9:57:27	597.45	0.05897	6.18471	0.002061	42.47
9:58:12	598.20	0.05895	6.18474	0.002061	42.58
9:58:57	598.95	0.05817	6.18029	0.002070	42.67
9:59:42	599.70	0.05817	6.19012	0.002050	42.44

10:00:27	600.45	0.05806	6.17055	0.002090	42.60
10:01:12	601.20	0.05853	6.17024	0.002091	42.50
10:01:57	601.95	0.05818	6.16507	0.002102	42.60
10:02:42	602.70	0.05803	6.15695	0.002119	42.52
10:03:27	603.45	0.05841	6.16677	0.002098	42.44
10:04:12	604.20	0.05834	6.17905	0.002072	42.46
10:04:57	604.95	0.05809	6.18810	0.002054	42.33
10:05:42	605.70	0.05850	6.17561	0.002080	42.33
10:06:27	606.45	0.05811	6.17649	0.002078	42.59
10:07:12	607.20	0.05830	6.17392	0.002083	42.27
10:07:57	607.95	0.05812	6.16869	0.002094	42.43
10:08:42	608.70	0.05841	6.16683	0.002098	42.54
10:09:27	609.45	0.05794	6.17283	0.002085	42.44
10:10:12	610.20	0.05784	6.17919	0.002072	42.44
10:10:57	610.95	0.05872	6.18487	0.002060	42.44
10:11:42	611.70	0.05809	6.18190	0.002067	42.45
10:12:27	612.45	0.05784	6.17639	0.002078	42.20
10:13:12	613.20	0.05793	6.18196	0.002066	42.52
10:13:57	613.95	0.05843	6.17271	0.002086	42.50
10:14:42	614.70	0.05812	6.18507	0.002060	42.53
10:15:27	615.45	0.05836	6.19637	0.002037	42.46
10:16:12	616.20	0.05886	6.18497	0.002060	42.59
10:16:57	616.95	0.05813	6.18393	0.002062	42.36
10:17:42	617.70	0.05811	6.19082	0.002048	42.25
10:18:27	618.45	0.05784	6.18156	0.002067	42.24
10:19:12	619.20	0.05872	6.18263	0.002065	42.21
10:19:57	619.95	0.05806	6.18945	0.002051	42.52
10:20:42	620.70	0.05771	6.17942	0.002072	42.27
10:21:25	621.42	0.05811	6.16989	0.002091	42.56
10:22:11	622.18	0.05835	6.17588	0.002079	42.39
10:22:56	622.93	0.05885	6.19092	0.002048	42.48
10:23:40	623.67	0.05791	6.18466	0.002061	42.49
10:24:25	624.42	0.05766	6.19240	0.002045	42.36
10:25:10	625.17	0.05785	6.18429	0.002062	42.49
10:25:56	625.93	0.05770	6.18396	0.002062	42.56

10:26:42	626.70	0.05853	6.17822	0.002074	42.55
10:27:27	627.45	0.05799	6.18380	0.002063	42.56
10:28:12	628.20	0.05775	6.17614	0.002078	42.52
10:28:57	628.95	0.05717	6.17365	0.002084	42.51
10:29:42	629.70	0.05706	6.17164	0.002088	42.35
10:30:27	630.45	0.05763	6.16706	0.002097	42.46
10:31:12	631.20	0.05688	6.14959	0.002134	42.24
10:31:57	631.95	0.05653	6.15989	0.002112	42.29
10:32:42	632.70	0.05727	6.16168	0.002109	42.18
10:33:27	633.45	0.05673	6.16363	0.002105	42.54
10:34:12	634.20	0.05724	6.15382	0.002125	42.42
10:34:57	634.95	0.05688	6.14821	0.002137	42.47
10:35:42	635.70	0.05707	6.15844	0.002116	42.48
10:36:27	636.45	0.05691	6.15259	0.002128	42.23
10:37:12	637.20	0.05660	6.14437	0.002146	42.33
10:37:57	637.95	0.05678	6.14753	0.002139	42.38
10:38:42	638.70	0.05668	6.14874	0.002136	42.25
10:39:27	639.45	0.05696	6.15574	0.002121	42.49
10:40:12	640.20	0.05673	6.13908	0.002157	42.18
10:40:57	640.95	0.05678	6.14514	0.002144	42.48
10:41:42	641.70	0.05681	6.15041	0.002133	42.34
10:42:27	642.45	0.05762	6.16583	0.002100	42.33
10:43:12	643.20	0.05702	6.16096	0.002110	42.17
10:43:57	643.95	0.05672	6.16205	0.002108	42.30
10:44:42	644.70	0.05619	6.15467	0.002124	42.28
10:45:27	645.45	0.05640	6.14705	0.002140	42.35
10:46:12	646.20	0.05597	6.14013	0.002155	42.47
10:46:57	646.95	0.05628	6.14010	0.002155	42.20
10:47:42	647.70	0.05741	6.14302	0.002148	42.35
10:48:27	648.45	0.05704	6.13834	0.002159	42.35
10:49:12	649.20	0.05555	6.13388	0.002168	42.27
10:49:57	649.95	0.05588	6.13311	0.002170	42.25
10:50:42	650.70	0.05633	6.13831	0.002159	42.12
10:51:27	651.45	0.05561	6.14213	0.002150	42.33
10:52:12	652.20	0.05700	6.13704	0.002161	42.17

10:52:57	652.95	0.05639	6.12575	0.002186	42.15
10:53:42	653.70	0.05608	6.13758	0.002160	42.22
10:54:27	654.45	0.05624	6.13198	0.002172	42.16
10:55:12	655.20	0.05615	6.13279	0.002171	42.19
10:55:57	655.95	0.05502	6.12342	0.002191	42.20
10:56:42	656.70	0.05639	6.12871	0.002179	42.16
10:57:27	657.45	0.05599	6.14286	0.002149	42.02
10:58:12	658.20	0.05718	6.14304	0.002148	42.13
10:58:57	658.95	0.05658	6.14345	0.002148	42.08
10:59:42	659.70	0.05684	6.14372	0.002147	42.14
11:00:27	660.45	0.05667	6.13993	0.002155	42.07
11:01:12	661.20	0.05681	6.14026	0.002154	42.07
11:01:57	661.95	0.05675	6.15388	0.002125	42.16
11:02:42	662.70	0.05657	6.14489	0.002144	42.18
11:03:27	663.45	0.05604	6.13996	0.002155	41.85
11:04:12	664.20	0.05634	6.13636	0.002163	42.03
11:04:57	664.95	0.05709	6.13937	0.002156	42.02
11:05:42	665.70	0.05570	6.13766	0.002160	41.86
11:06:27	666.45	0.05583	6.13555	0.002165	41.89
11:07:12	667.20	0.05646	6.13408	0.002168	41.84
11:07:57	667.95	0.05606	6.13220	0.002172	41.89
11:08:42	668.70	0.05668	6.13926	0.002157	41.92
11:09:27	669.45	0.05634	6.15237	0.002128	41.65
11:10:12	670.20	0.05582	6.14168	0.002151	42.02
11:10:57	670.95	0.05680	6.14212	0.002150	41.80
11:11:42	671.70	0.05716	6.14134	0.002152	41.67
11:12:27	672.45	0.05561	6.13536	0.002165	41.56
11:13:12	673.20	0.05613	6.14066	0.002153	41.61
11:13:57	673.95	0.05651	6.14003	0.002155	41.91
11:14:42	674.70	0.05658	6.13974	0.002155	41.78
11:15:27	675.45	0.05541	6.12841	0.002180	41.74
11:16:12	676.20	0.05575	6.12101	0.002196	41.81
11:16:57	676.95	0.05744	6.12490	0.002188	41.78
11:17:42	677.70	0.05683	6.11538	0.002209	41.71
11:18:27	678.45	0.05733	6.10932	0.002222	41.67

11:19:12	679.20	0.05638	6.09767	0.002248	41.88
11:19:57	679.95	0.05653	6.09348	0.002258	41.77
11:20:42	680.70	0.05609	6.08579	0.002275	41.83
11:21:27	681.45	0.05571	6.09200	0.002261	41.92
11:22:12	682.20	0.05525	6.09005	0.002265	41.67
11:22:57	682.95	0.05535	6.08116	0.002286	41.82
11:23:42	683.70	0.05595	6.08624	0.002274	41.56
11:24:27	684.45	0.05551	6.08007	0.002288	41.67
11:25:12	685.20	0.05617	6.07104	0.002309	41.59
11:25:57	685.95	0.05543	6.07222	0.002306	41.39
11:26:42	686.70	0.05532	6.07038	0.002310	41.64
11:27:27	687.45	0.05504	6.06959	0.002312	41.75
11:28:12	688.20	0.05474	6.06951	0.002312	41.64
11:29:02	689.03	0.05475	6.08874	0.002268	41.62
11:29:54	689.90	0.05437	6.09293	0.002259	41.80
11:30:45	690.75	0.05499	6.09930	0.002244	41.73
11:31:37	691.62	0.05372	6.09855	0.002246	41.58
11:32:19	692.32	0.05455	6.08901	0.002268	41.72
11:32:28	692.47	0.05474	6.08687	0.002273	41.76
11:33:20	693.33	0.05409	6.09287	0.002259	41.31
11:33:33	693.55	0.05378	6.10610	0.002229	41.57
11:33:48	693.80	0.05500	6.09669	0.002250	41.57
11:34:04	694.07	0.05295	6.11981	0.002199	41.43
11:34:19	694.32	0.05432	6.09857	0.002246	41.56
11:34:33	694.55	0.05443	6.09533	0.002253	41.39
11:34:48	694.80	0.05360	6.10981	0.002221	41.43
11:35:03	695.05	0.05310	6.10317	0.002236	41.42
11:35:18	695.30	0.05440	6.09871	0.002246	41.57
11:35:32	695.53	0.05673	6.11651	0.002206	41.43

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